

Kelthane–Dicofol 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>

Prepared: 2016–06–15 13:50:48
SpecLibDDT version
OrgMassSpecR version 0.4–4
R version 3.3.0 (2016–05–03)

Name: chlorodiphenyl-methanone

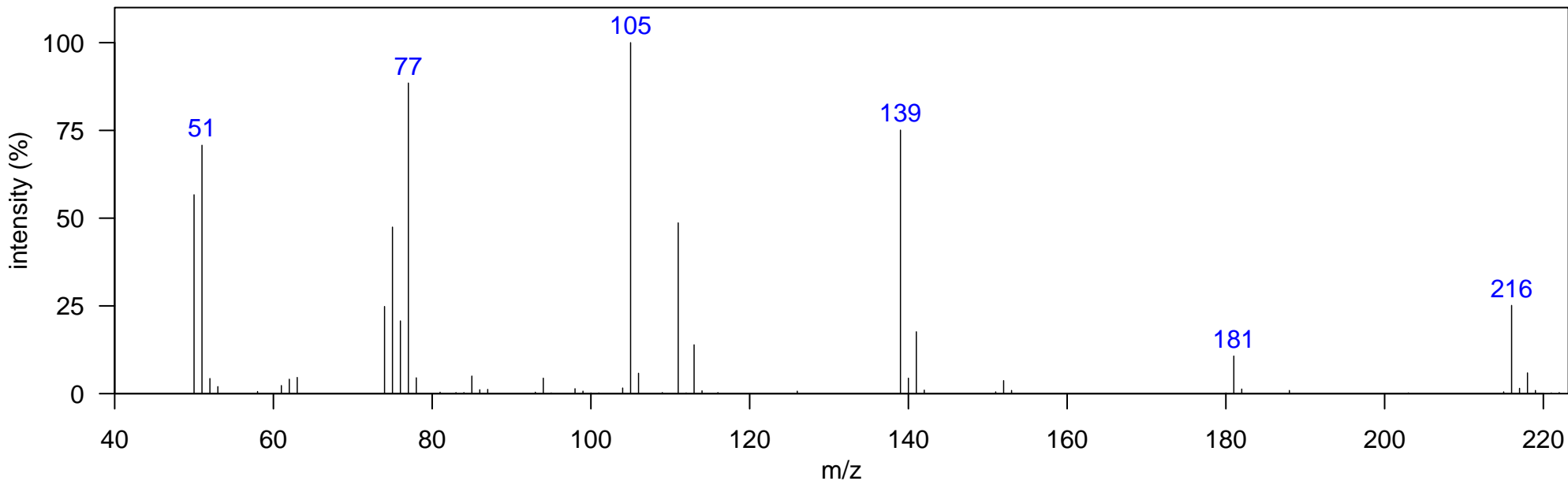
Technical Mixture: Kelthane 500PPM

Compound Class: other

Elemental Formula: C₁₃H₉ClO

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. (4-chlorophenyl)phenyl-methanone



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 chlorodiphenyl-methanone	FALSE	FALSE	1177.17	1.135

m/z [Fragment]
139 [M-C ₆ H ₅ Cl] ⁺
181 [M-Cl] ⁺
216 M ⁺

Name: DDM

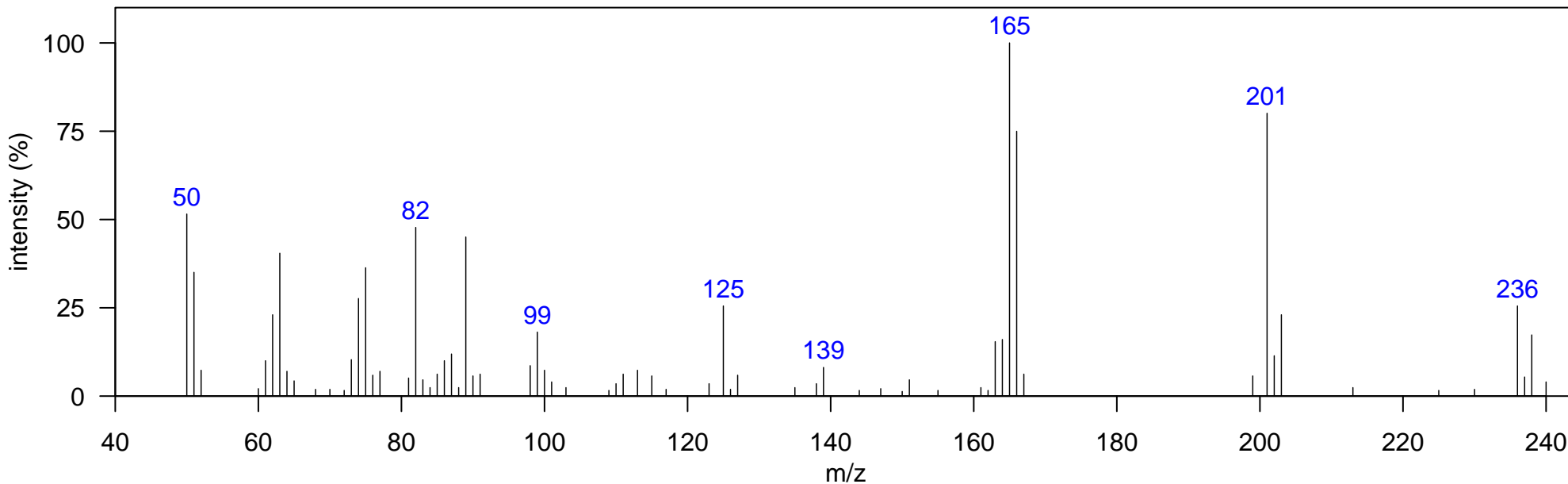
Technical Mixture: Kelthane 500PPM

Compound Class: known DDT 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 p,p'-DDM	TRUE	FALSE	1208.65	1.109

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

Name: DBP

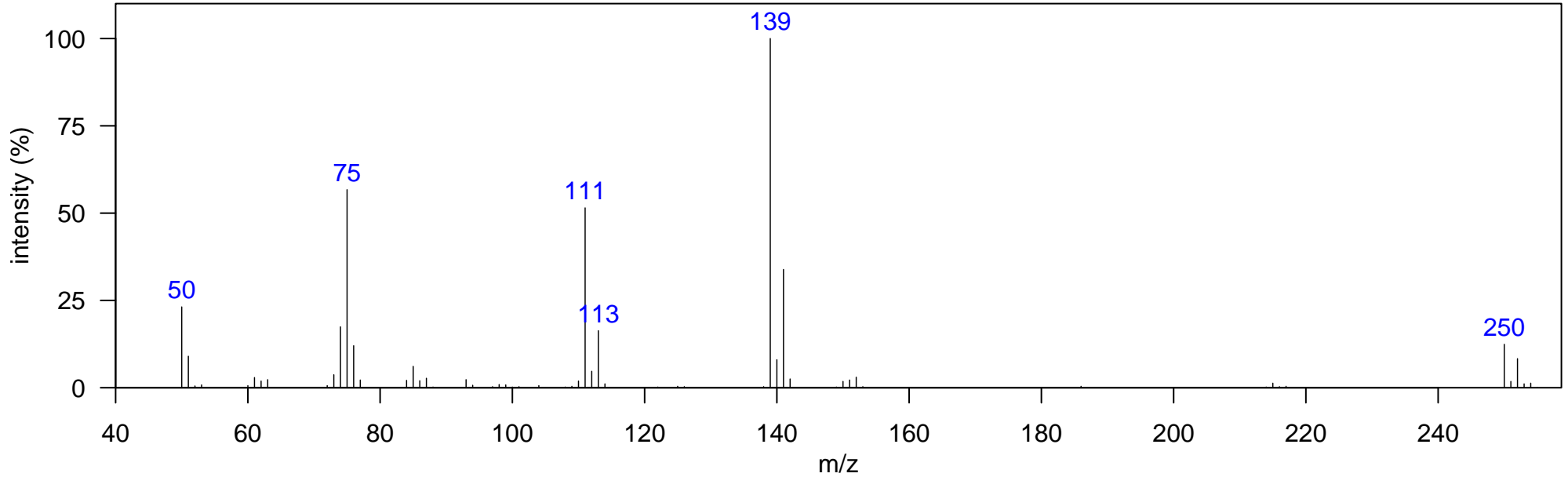
Technical Mixture: Kelthane 500PPM

Compound Class: known DDT degradation product

Elemental Formula: C₁₃H₈Cl₂O

Instrument: GCxGC-TOF, EI, 70 eV

Comment: Potential GC-inlet degradation product of dicofol.



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	o,p'-DBP	FALSE	FALSE	1254.13	1.195
2	DBP 1	FALSE	FALSE	1275.11	1.155
3	p,p'-DBP	TRUE	FALSE	1289.11	1.181
4	DBP 2	FALSE	FALSE	1338.08	1.089

m/z [Fragment]

75 [M-C₇H₅Cl₂O]⁺
111 [M-C₇H₄ClO]⁺
139 [M-C₆H₄Cl]⁺
250 M⁺

Name: DDOH

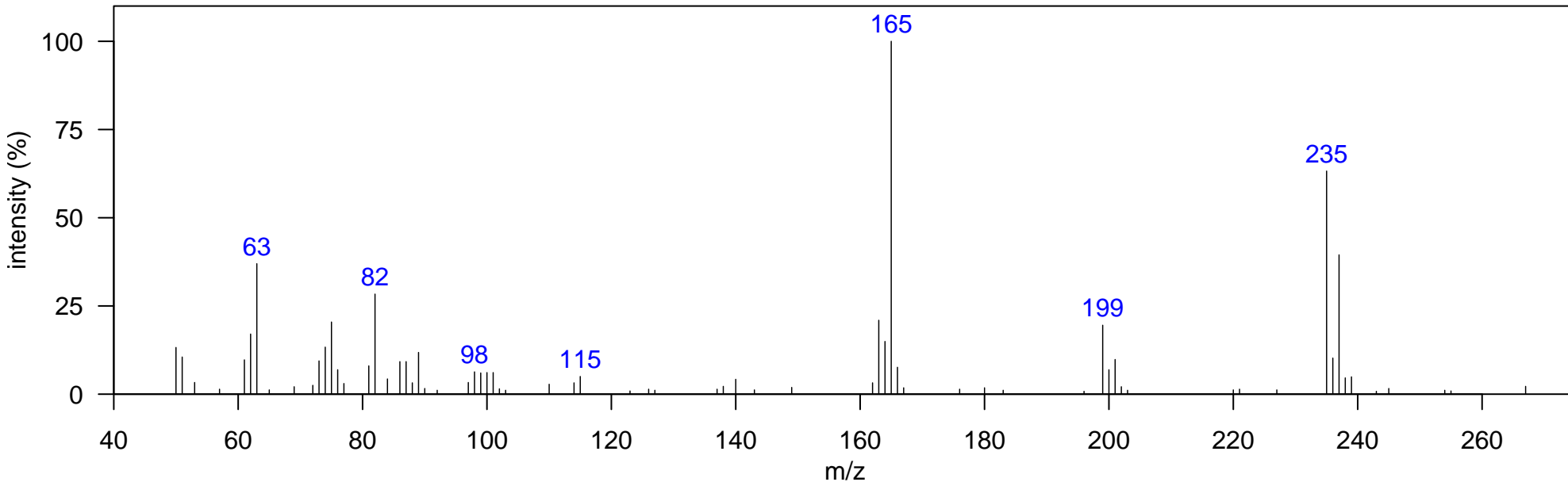
Technical Mixture: Kelthane 500PPM

Compound Class: known DDT degradation product

Elemental Formula: C₁₄H₁₂Cl₂O

Instrument: GCxGC-TOF, EI, 70 eV

Comment: NIST I.D. 2,2-Bis(p-chlorophenyl)ethanol



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDOH	FALSE	FALSE	1334.58 1.188

m/z [Fragment]

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

Name: DDE

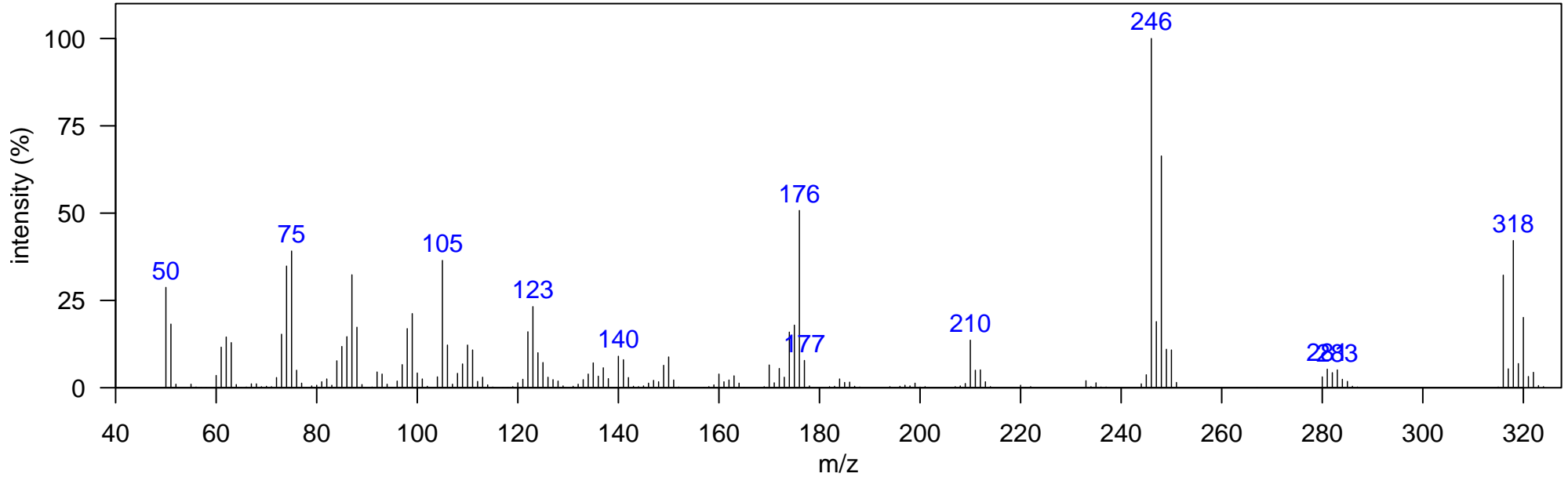
Technical Mixture: Kelthane 500PPM

Compound Class: known major DDT degradation product

Elemental Formula: C₁₄H₈Cl₄

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	o,p'-DDE	TRUE	TRUE	1352.07	1.168
2	DDE 1	FALSE	FALSE	1369.56	1.155
3	p,p'-DDE	TRUE	TRUE	1383.55	1.168
4	DDE 2	FALSE	FALSE	1408.04	1.135
5	DDE 3	FALSE	FALSE	1551.46	1.016

m/z [Fragment]

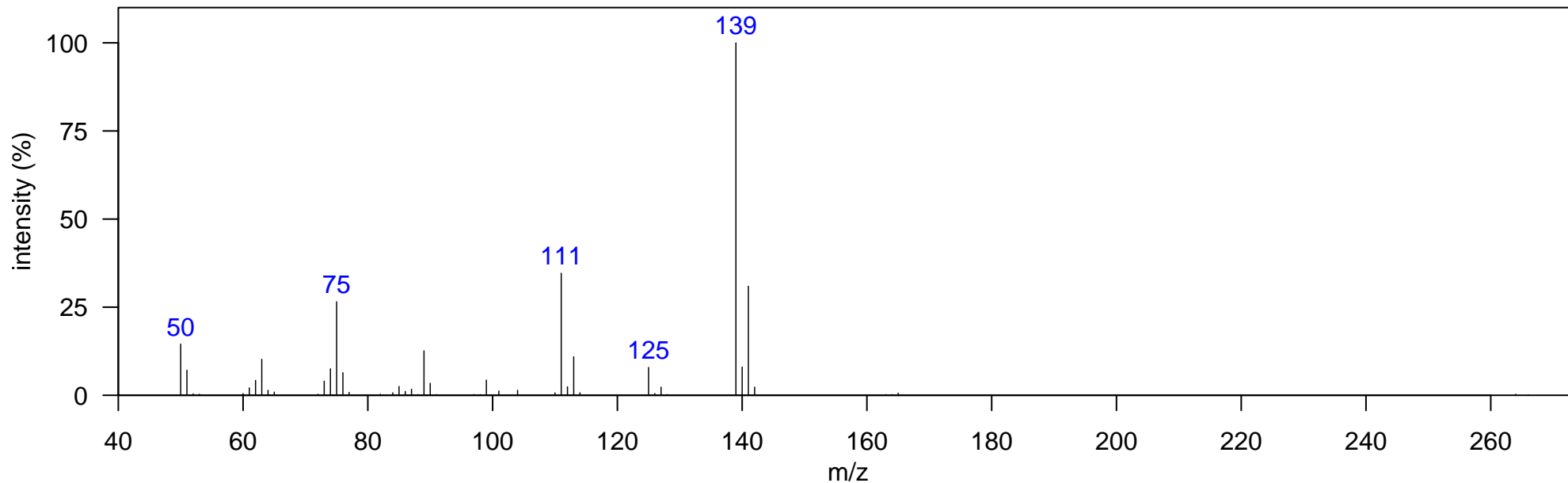
176 [M-Cl₄]⁺
211 [M-Cl₃]⁺
246 [M-Cl₂]⁺
281 [M-Cl]⁺
316 M⁺

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



m/z [Fragment]

Isomer Information

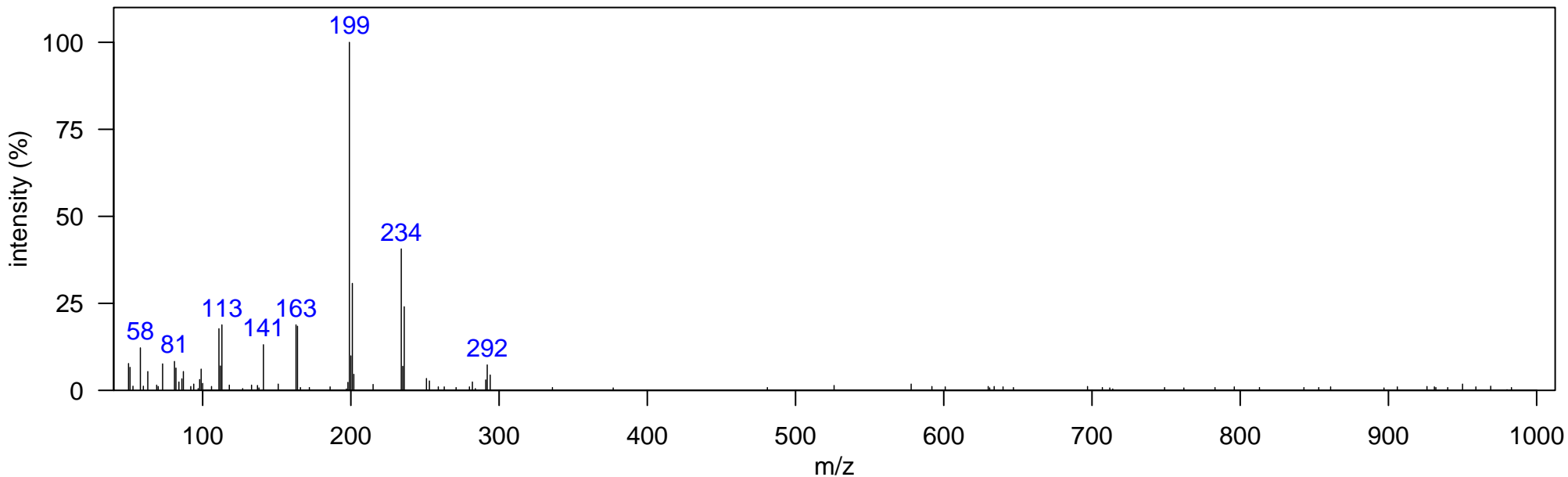
	Isomer	InDolphin	Monitored	RT1D	RT2D
1	unknown 1-1	FALSE	FALSE	1359.07	1.214
2	unknown 1-2	FALSE	FALSE	1390.55	1.168
3	unknown 1-3	FALSE	FALSE	1415.03	1.188
4	unknown 1-4	FALSE	FALSE	1418.53	1.129
5	unknown 1-5	FALSE	FALSE	1418.53	1.234
6	unknown 1-6	FALSE	FALSE	1422.03	1.181

Compound Class: other

Elemental Formula:

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1 unknown 2	FALSE	FALSE	1422.03	1.168

m/z [Fragment]

m/z [Fragment]

Name: DDMU

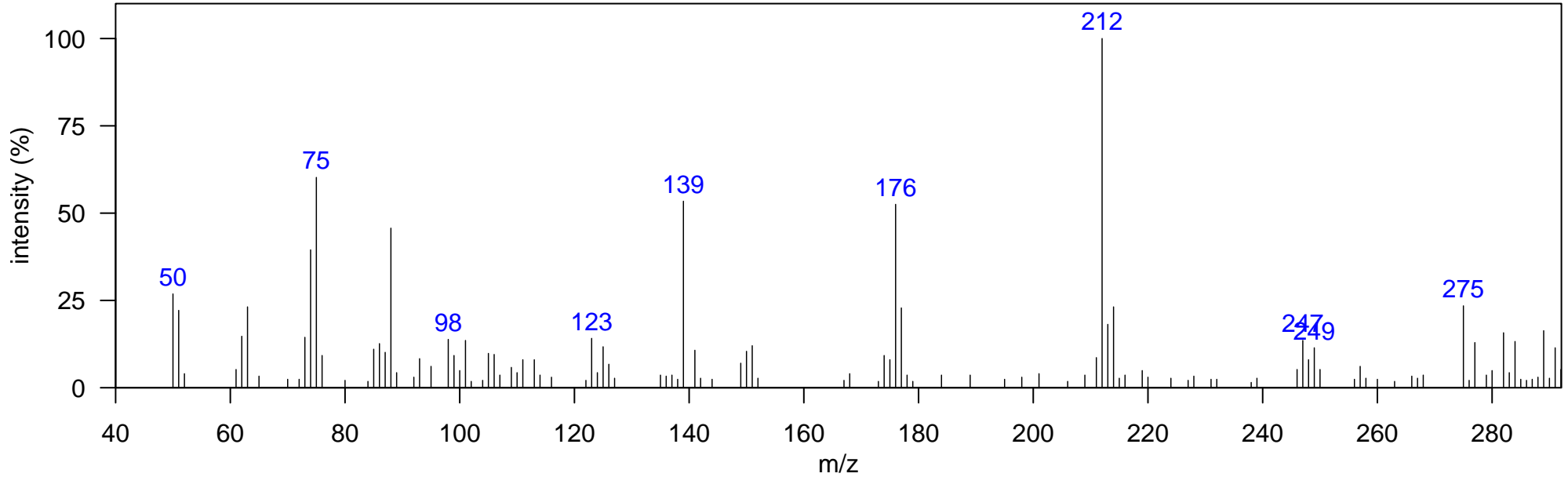
Technical Mixture: Kelthane 500PPM

Compound Class: known DDT degradation product

Elemental Formula: C₁₄H₉Cl₃

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

Isomer	InDolphin	Monitored	RT1D	RT2D
1	DDMU	FALSE	FALSE	1425.53 1.214

m/z [Fragment]
176 [M-HCl ₃] ⁺
212 [M-Cl ₂] ⁺
247 [M-Cl] ⁺
282 M ⁺

Name: DDT

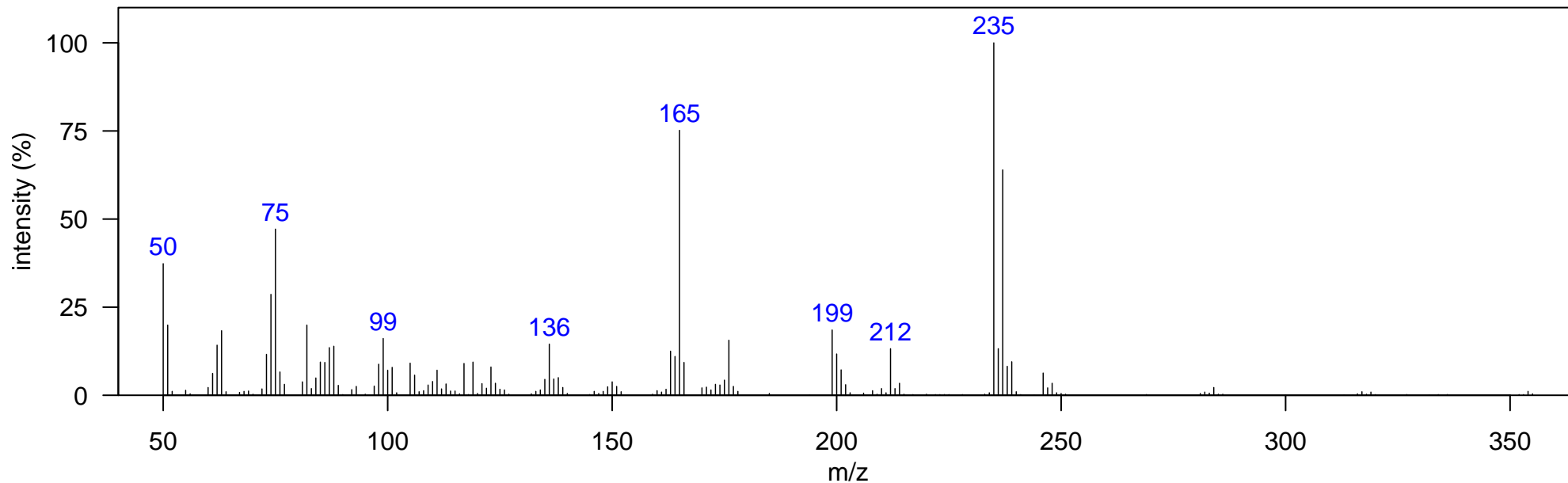
Technical Mixture: Kelthane 500PPM

Compound Class: DDT

Elemental Formula: C₁₄H₉Cl₅

Instrument: GCxGC-TOF, EI, 70 eV

Comment:



Isomer Information

	Isomer	InDolphin	Monitored	RT1D	RT2D
1	o,p'-DDT	TRUE	TRUE	1436.02	1.228
2	p,p'-DDT	TRUE	TRUE	1471.00	1.234

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