Kelthane−Dicofol Technical Mixture (500 ppm)

40 Years After The Ban: DDT−Related Compounds Accumulating in Southern California Bottlenose Dolphins

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

Prepared: 2015−03−16 12:29:02
SpecLibDDT version
OrgMassSpecR version 0.4−4
R version 3.1.0 (2014−04−10)

Name: chlorodiphenyl−methanone

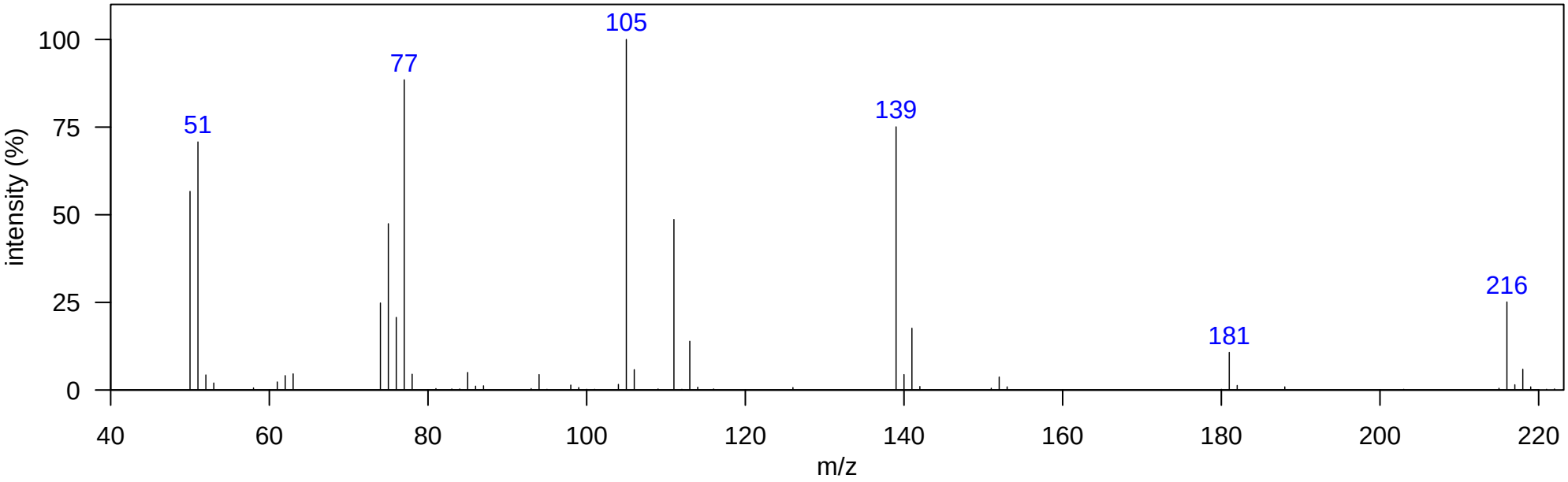
Technical Mixture: Kelthane 500PPM

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−C6H5Cl]+
181 [M−Cl]+
216 M+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DDM

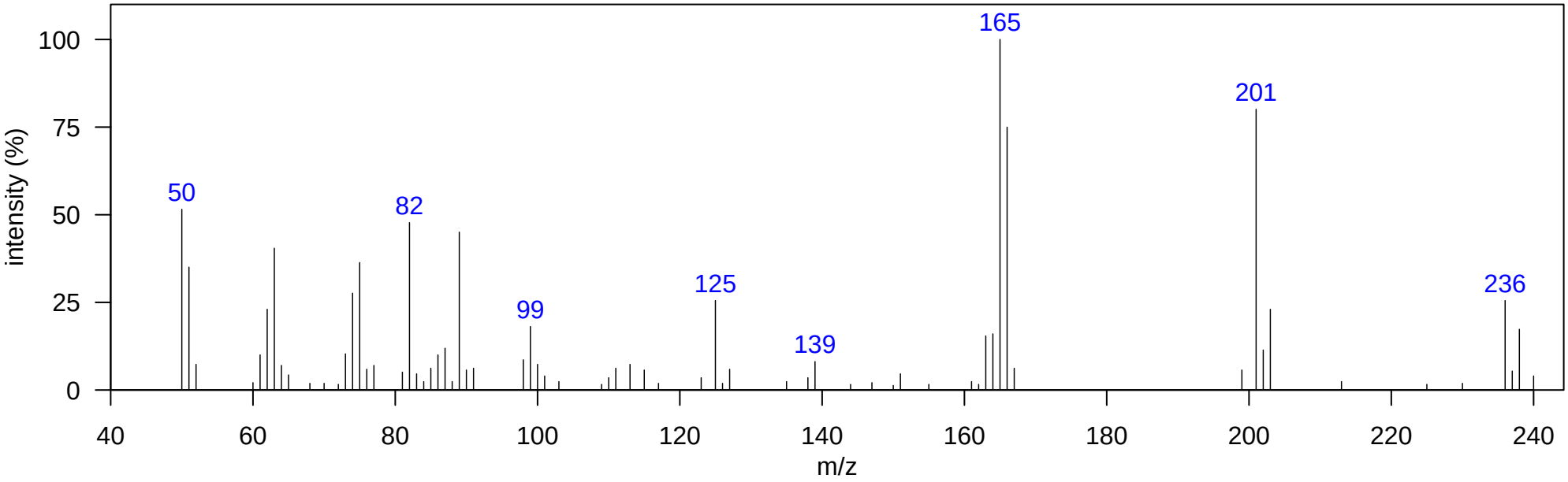
Technical Mixture: Kelthane 500PPM

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−HCl2]+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DBP

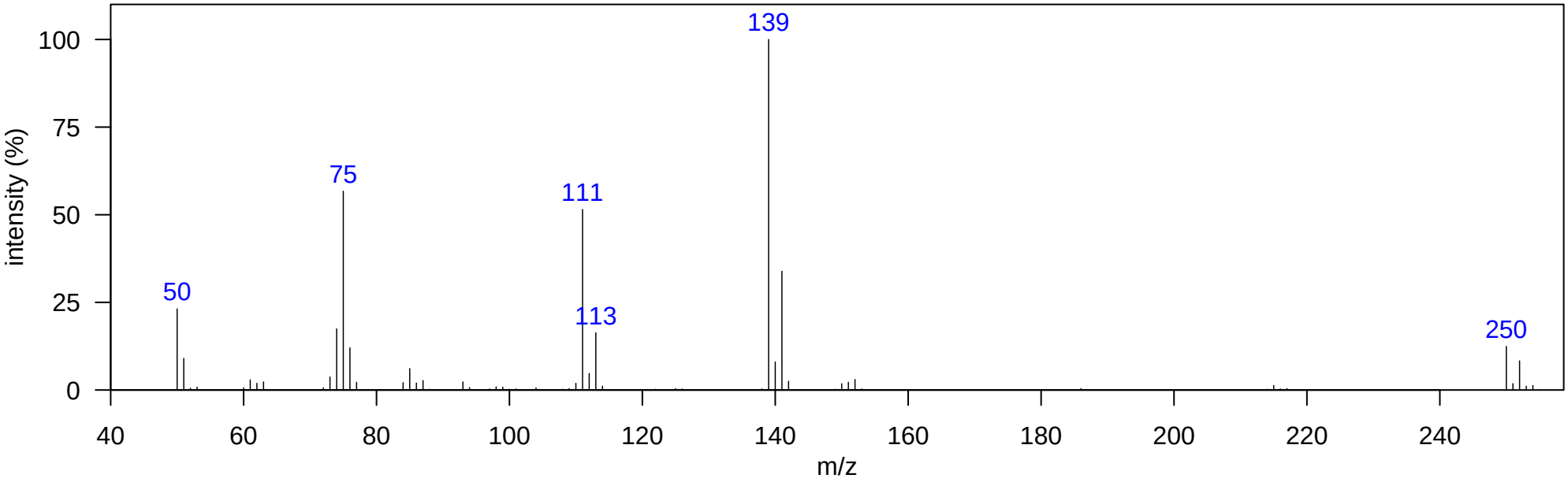
Technical Mixture: Kelthane 500PPM

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+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DDOH

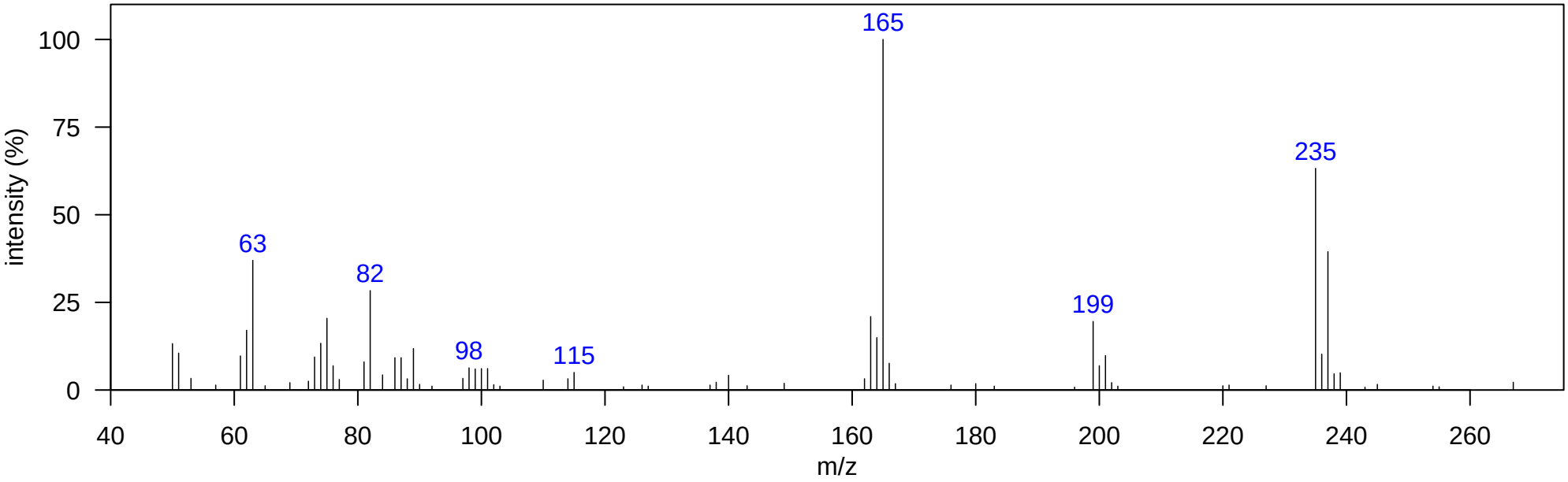
Technical Mixture: Kelthane 500PPM

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−CH4Cl2O]+
199 [M−CH4ClO]+
235 [M−CH3O]+
266 M+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DDE

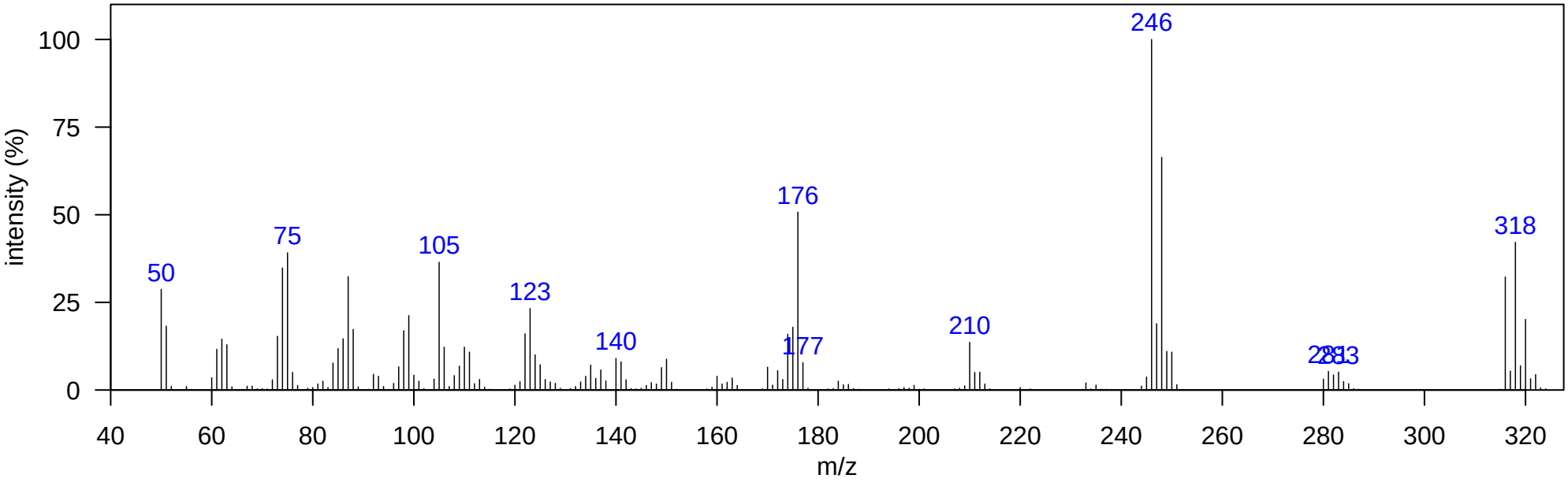
Technical Mixture: Kelthane 500PPM

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+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: unknown 1

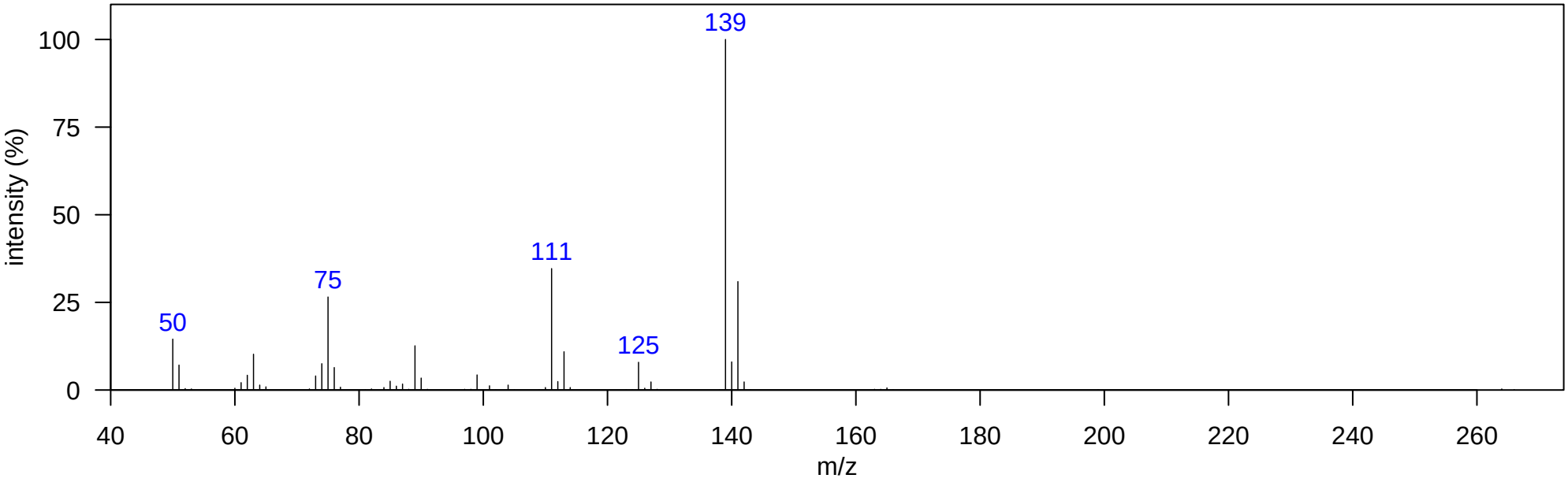
Technical Mixture: Kelthane 500PPM

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	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

m/z [Fragment]

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: unknown 2

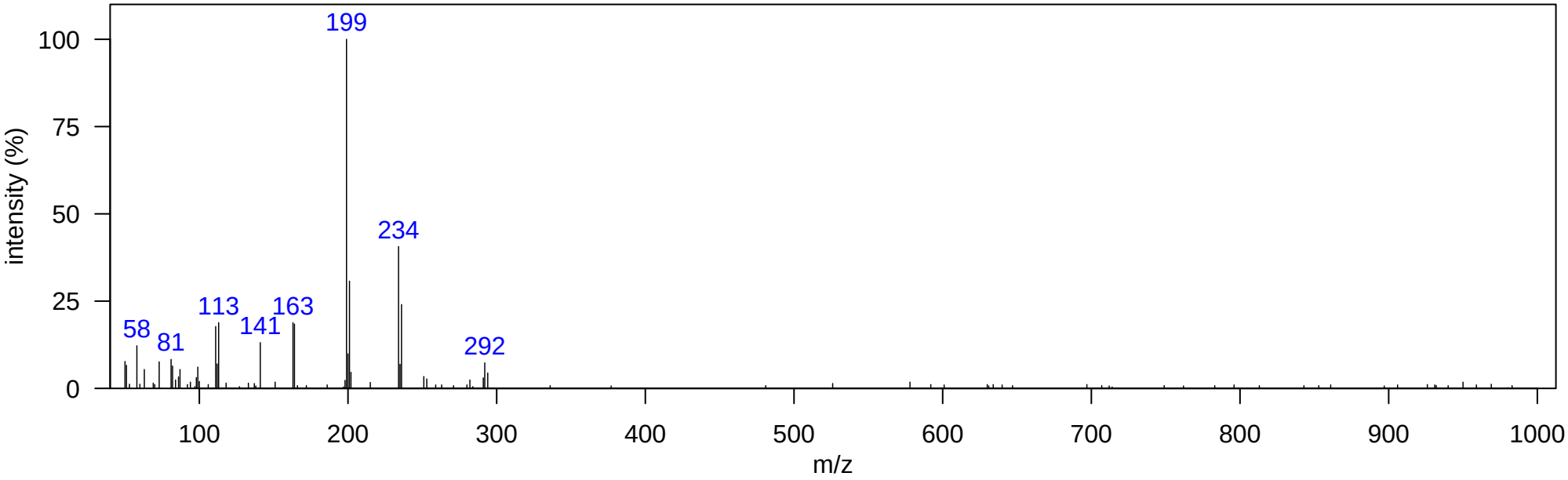
Technical Mixture: Kelthane 500PPM

Compound Class: other

Instrument: GCxGC−TOF, EI, 70 eV

Comment:

Elemental Formula:



Isomer Information

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

m/z [Fragment]

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DDMU

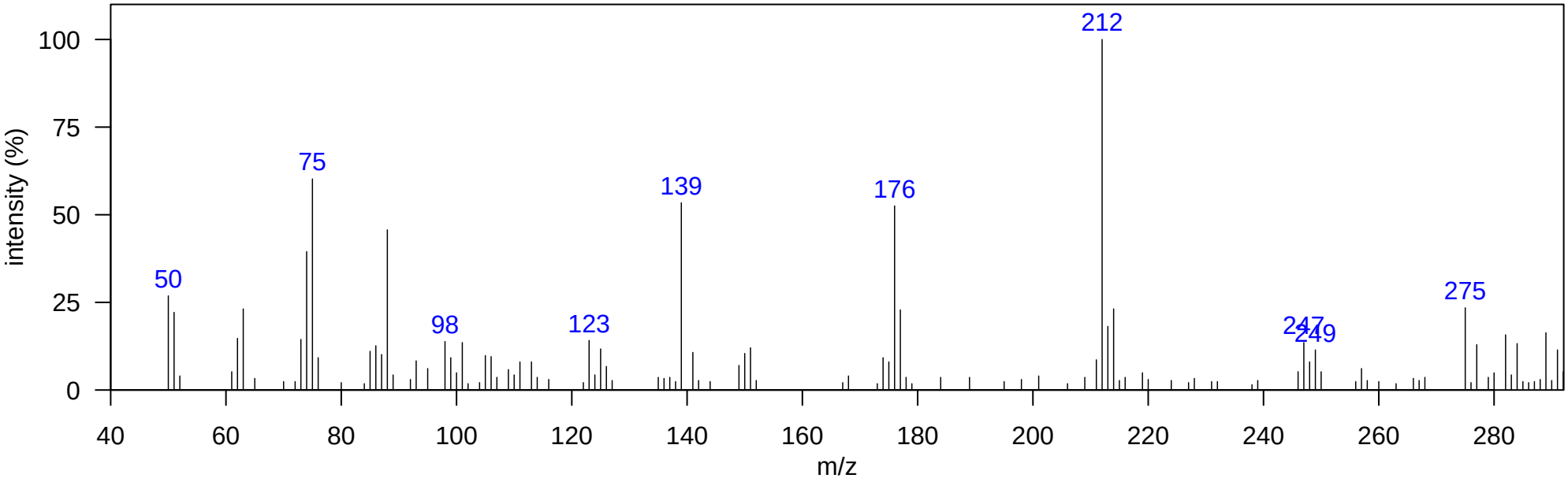
Technical Mixture: Kelthane 500PPM

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−HCl3]+
212 [M−Cl2]+
247 [M−Cl]+
282 M+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times

Name: DDT

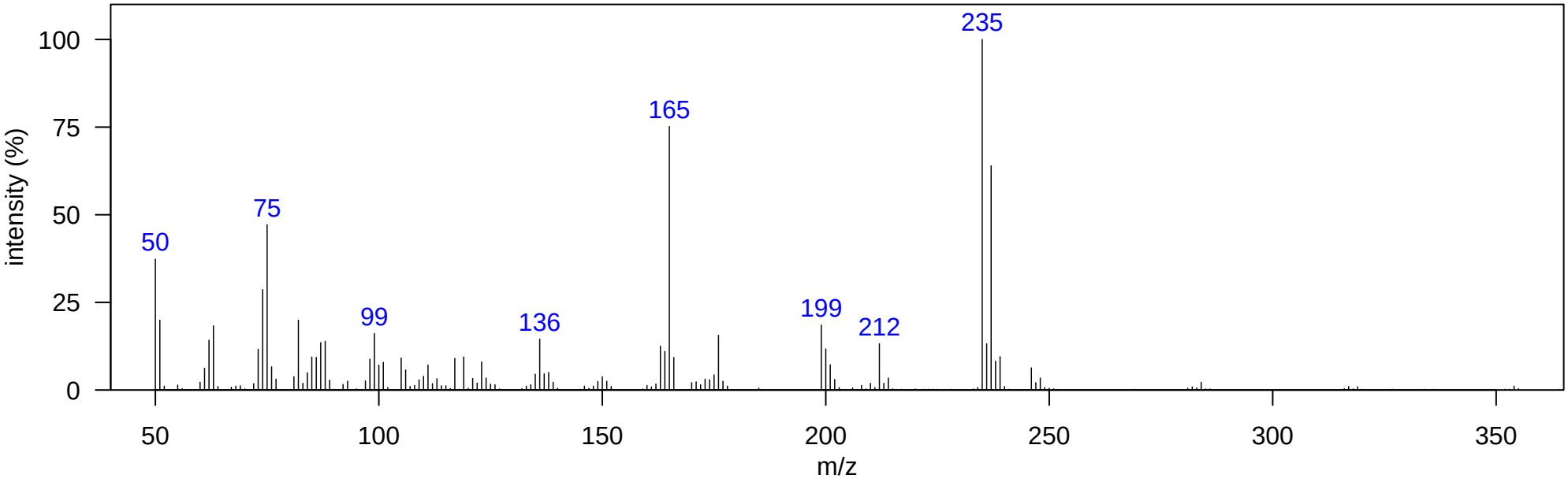
Technical Mixture: Kelthane 500PPM

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−CH2Cl3]+
354 M+

InDolphin = In Pacific Dolphin (Shaul, et al., 2015); Monitored = Typically Monitored; RT1D and RT2D = 1st and 2nd Dimension Retention Times