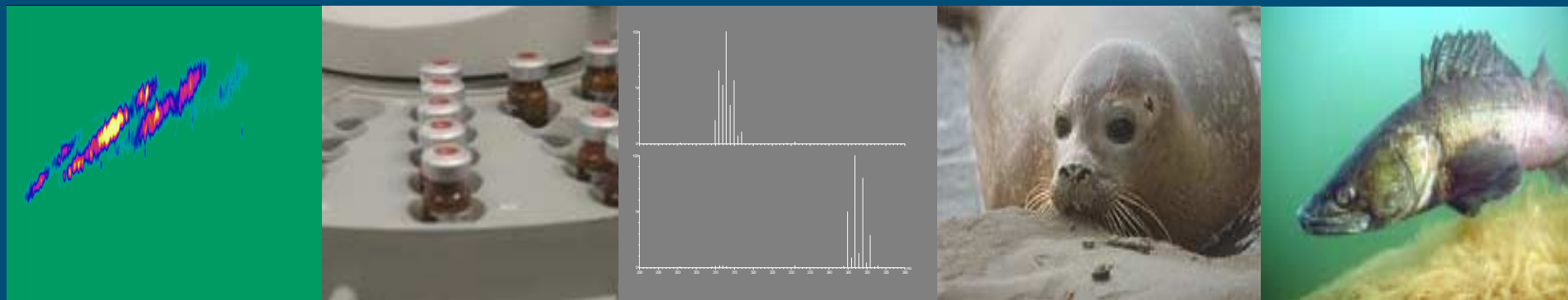


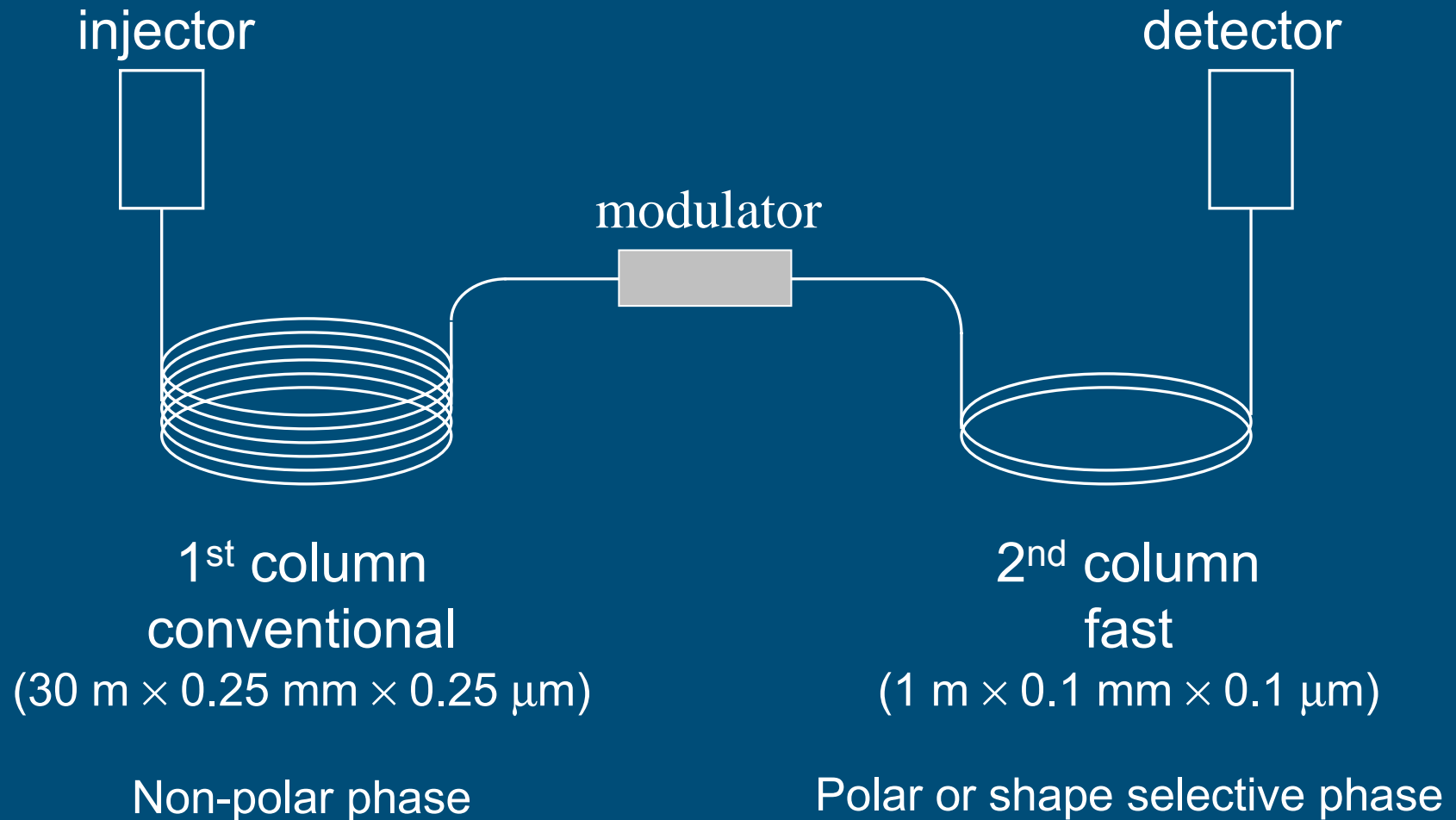
Quadrupole MS as detector for GCxGC

Peter Korytár

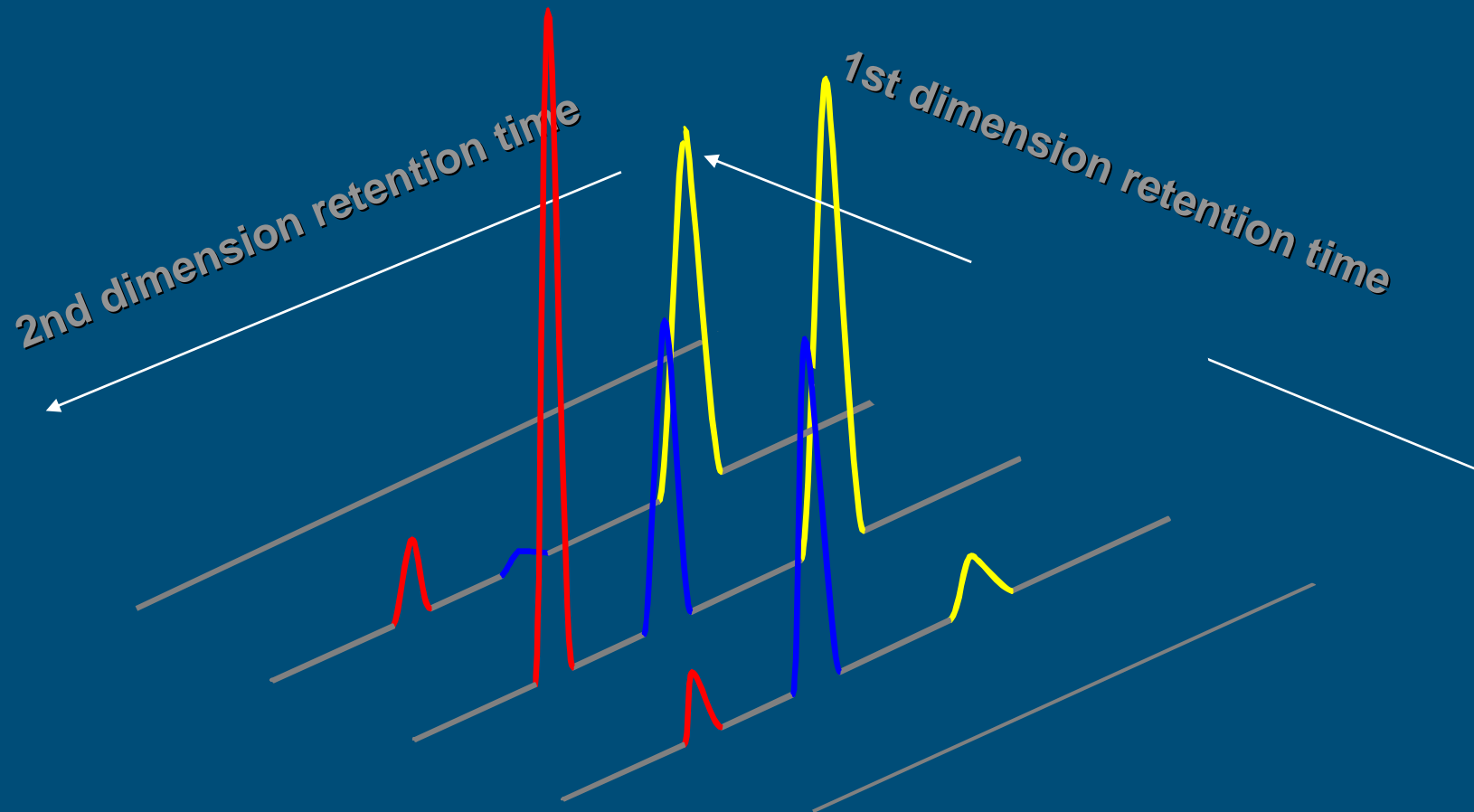
Netherlands Institute for Fisheries Research, IJmuiden, The Netherlands



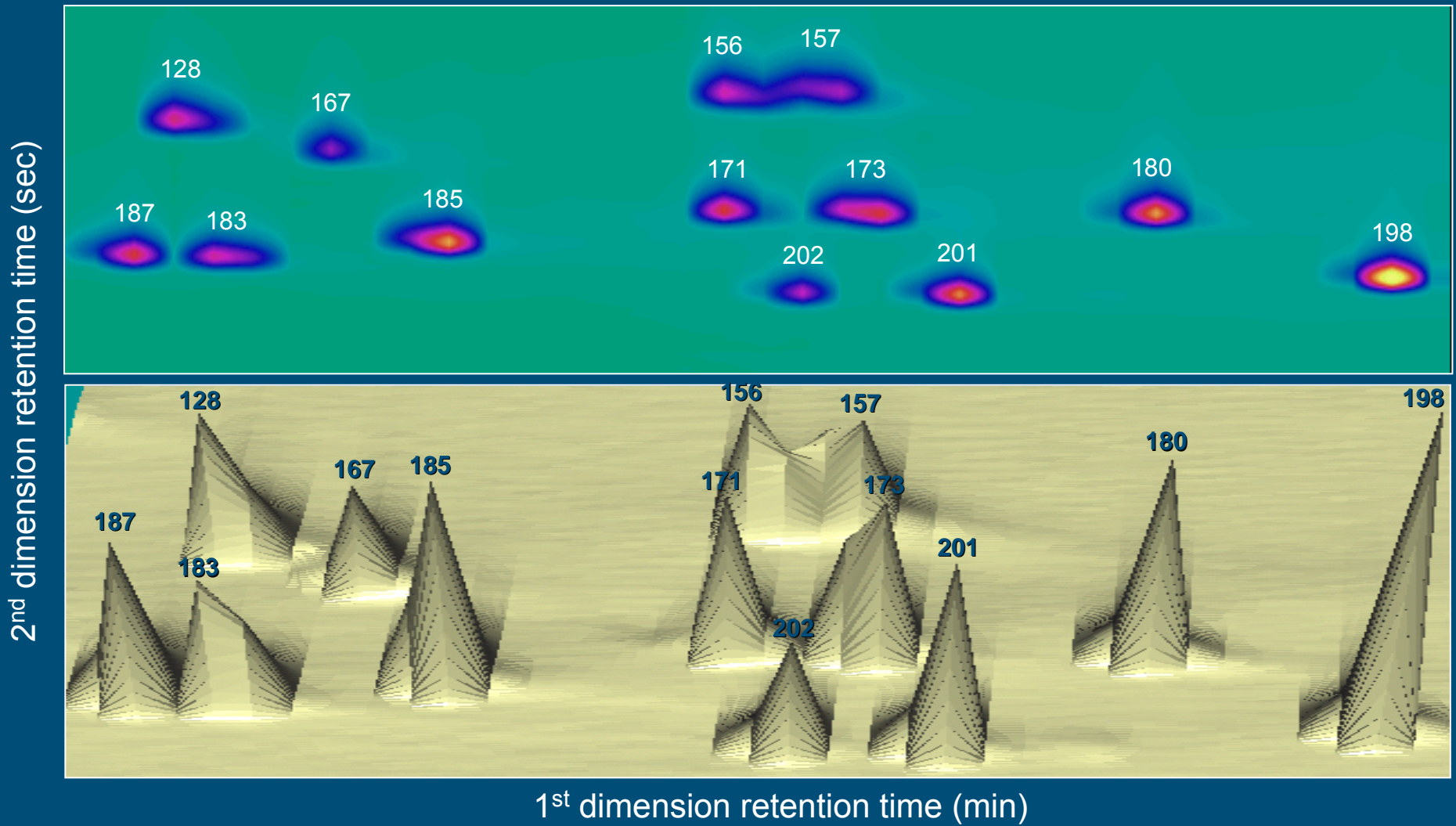
GC×GC principle



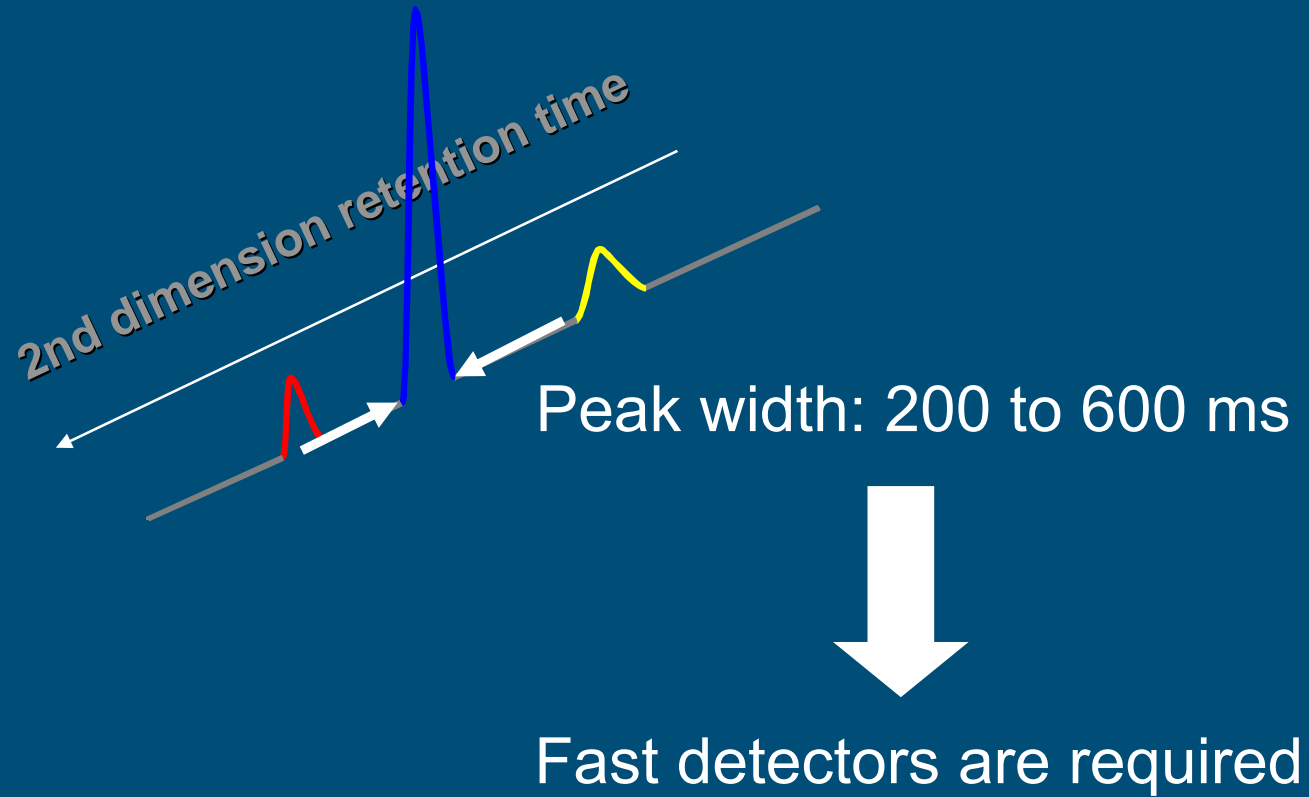
GC×GC principle



GC×GC principle



Instrument requirements

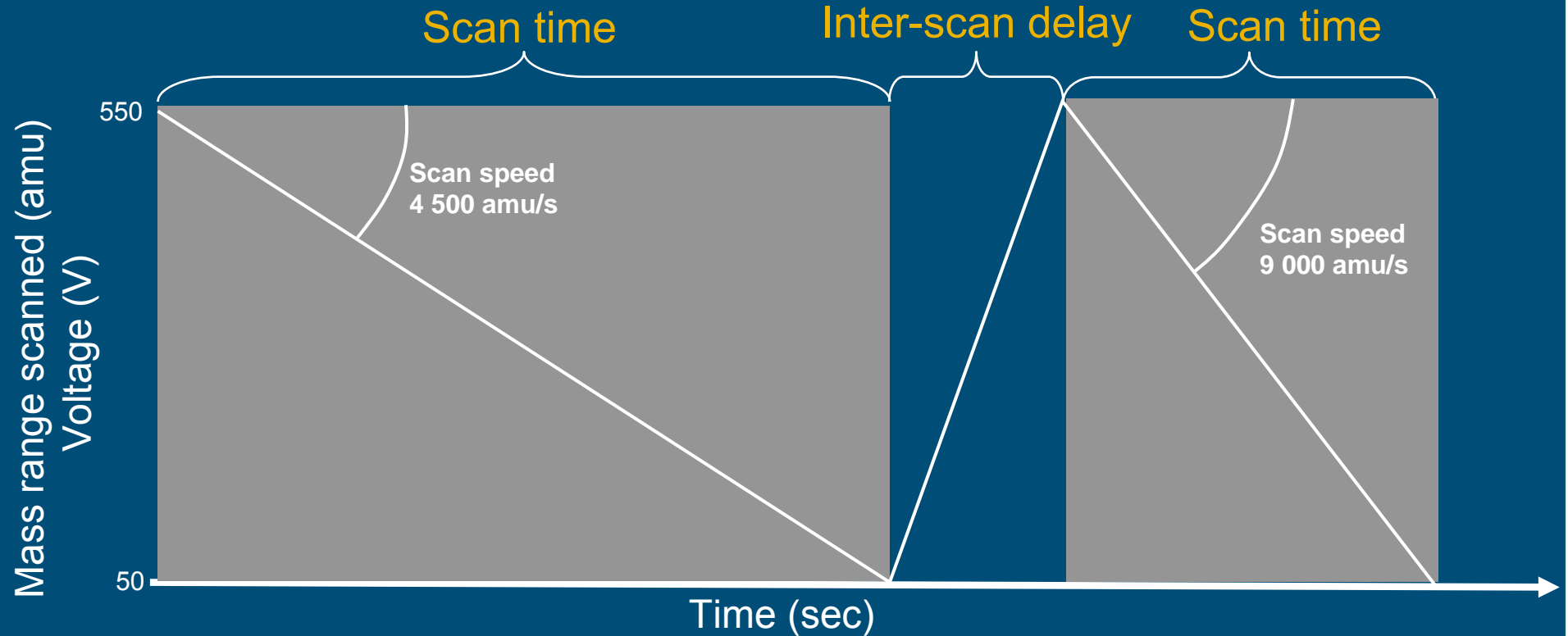


Objectives

- What are the capabilities of PerkinElmer qMS equipped with EI and CI mode as detector for GC × GC ?
 - Scan mode
 - Selected ion recording
- Is GC × GC – qMS NCI suitable for analysis of
 - Polychlorinated alkanes
 - PBDEs
 - PCDDs and PCDFs



Data acquisition rate in scan mode



$$\text{Data acquisition rate (Hz)} = \frac{1}{\text{Scan time (sec)} + \text{Inter-scan delay (sec)}}$$

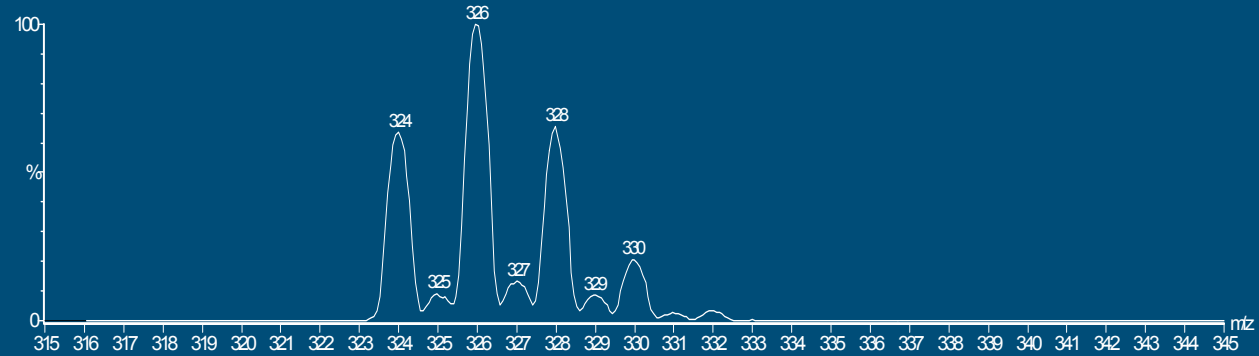


Influence of scan speed

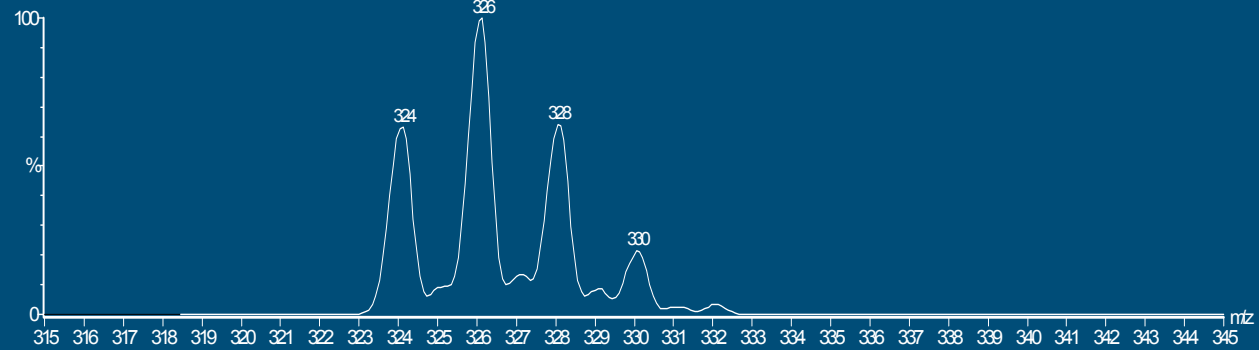
CB 126

Average continuum mass spectra

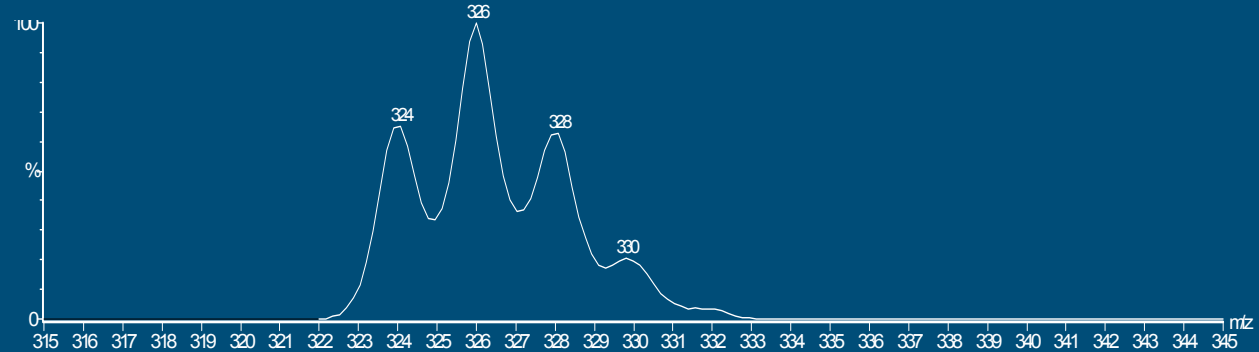
3 500 Da/s



8 750 Da/s

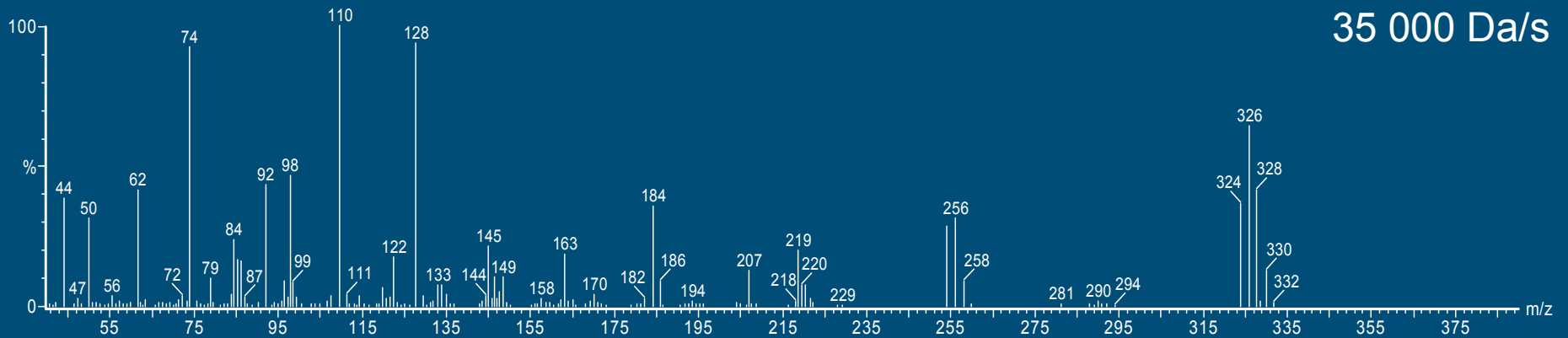
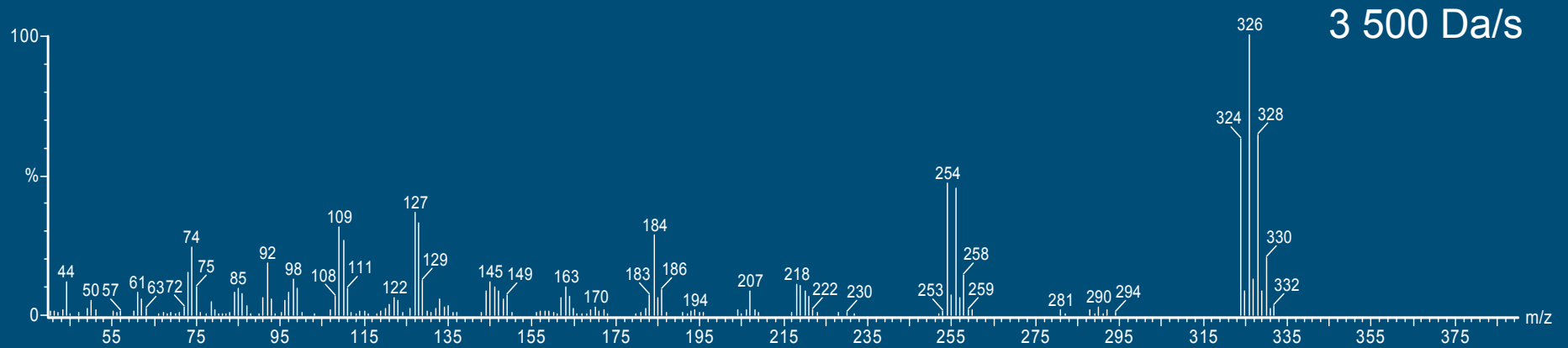


35 000 Da/s



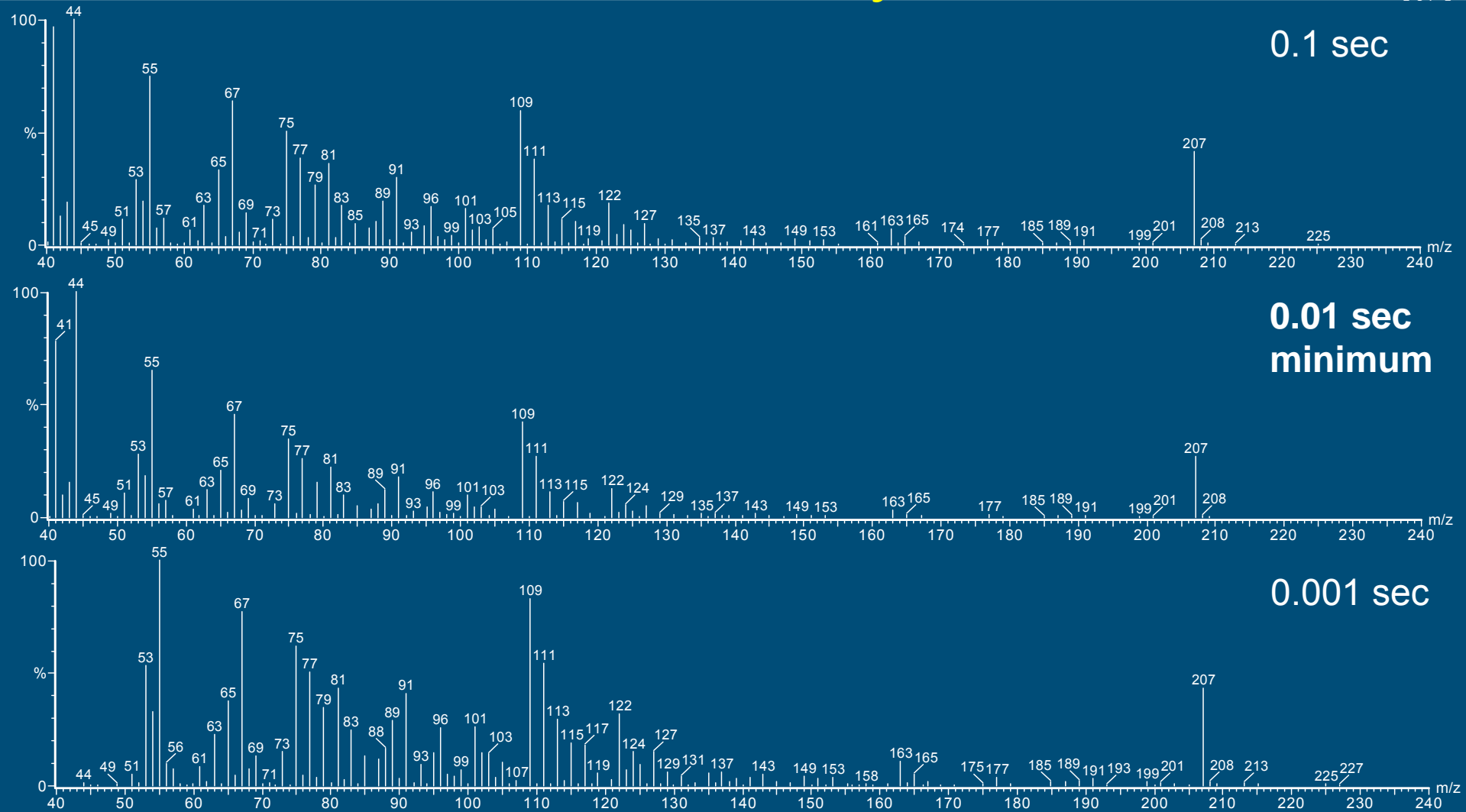
Influence of scan speed

CB 126, mass range 350 Da



Influence of inter-scan delay

Octachloro-undecane
Mass range 200 Da



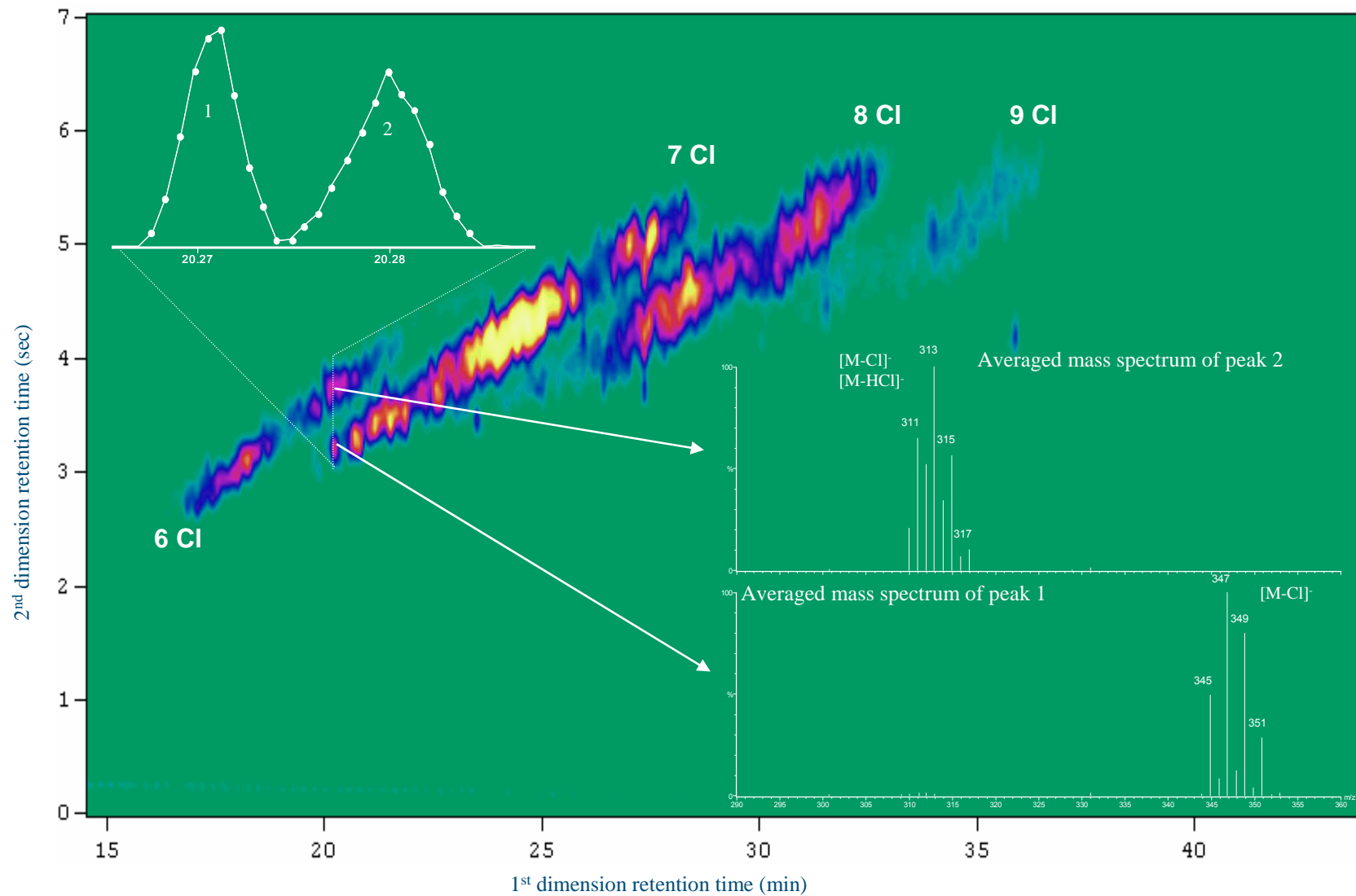
Capability of qMS in scan mode

Mass Range Scanned (Da)	Minimum inter-scan Delay (sec)	Maximum Data Acquisition rate at 9000 Da/s (Hz)	Detectable Peak width at 9000 Da/s (ms)*
400	0.014	17	400
300	0.011	23	300
200	0.010	33	210
100	0.005	62	112
50	0.001	152	49

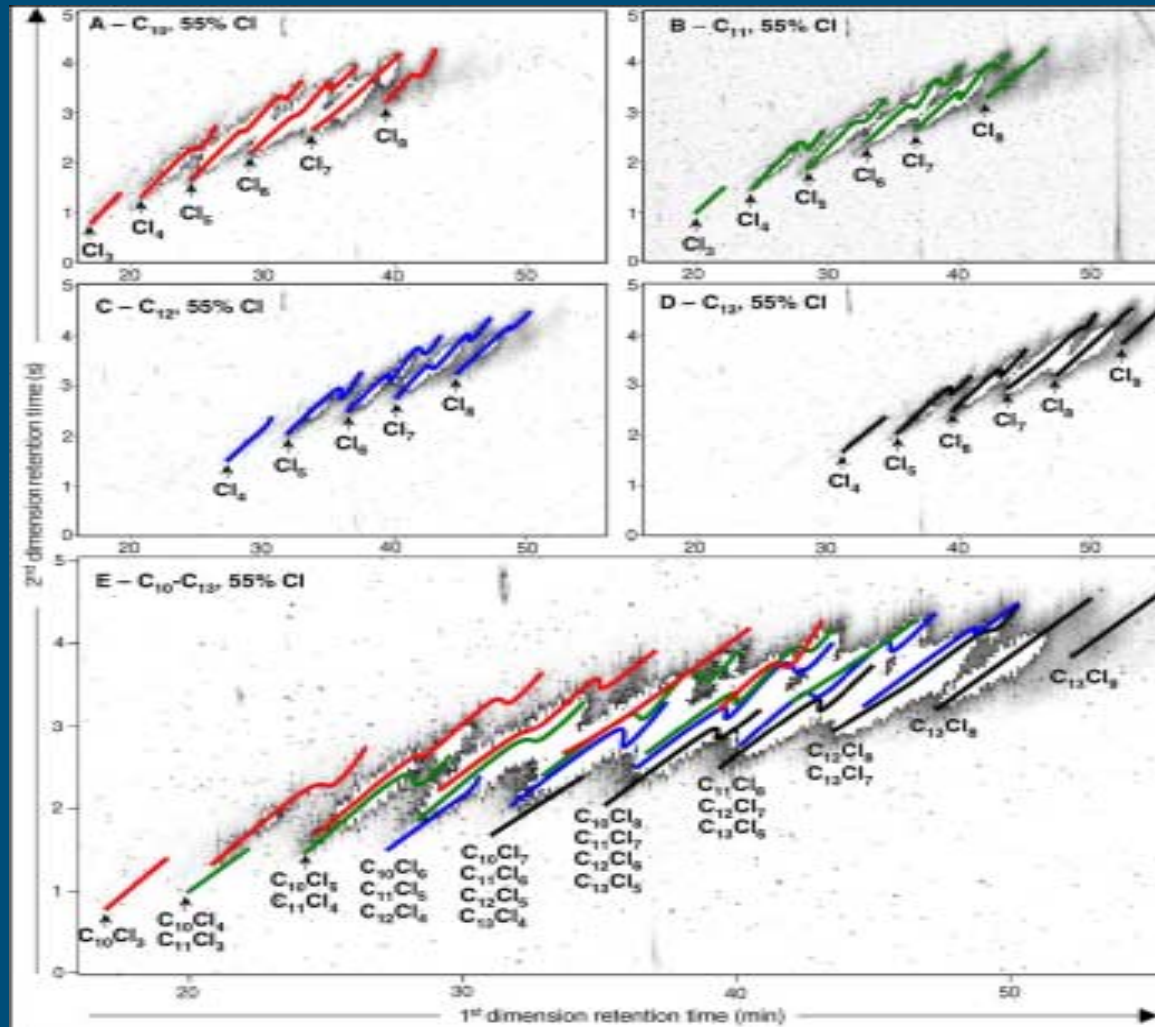
* calculated for 7 points per peak



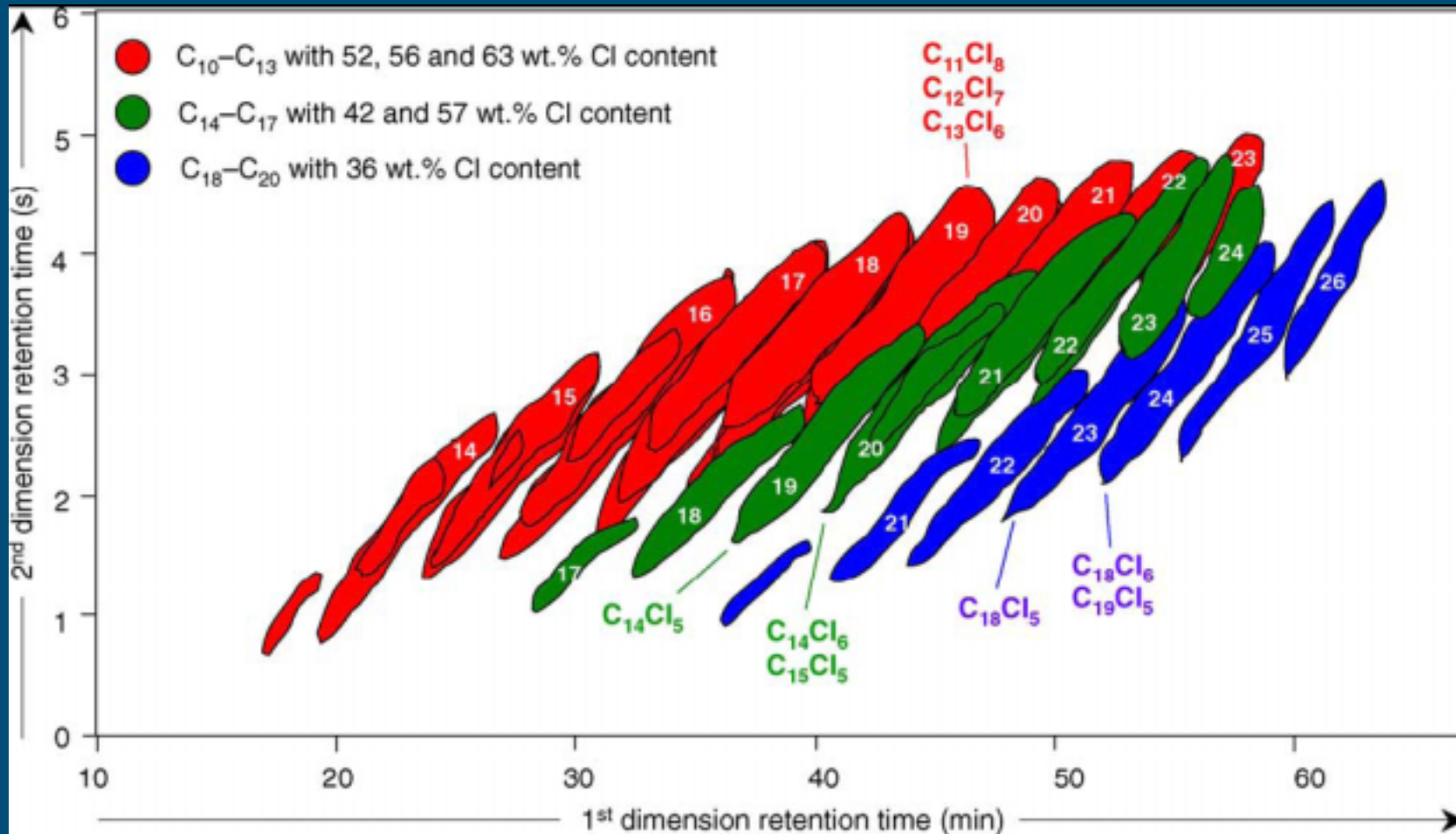
GCxGC-NCI MS chromatogram of polychlorinated decanes



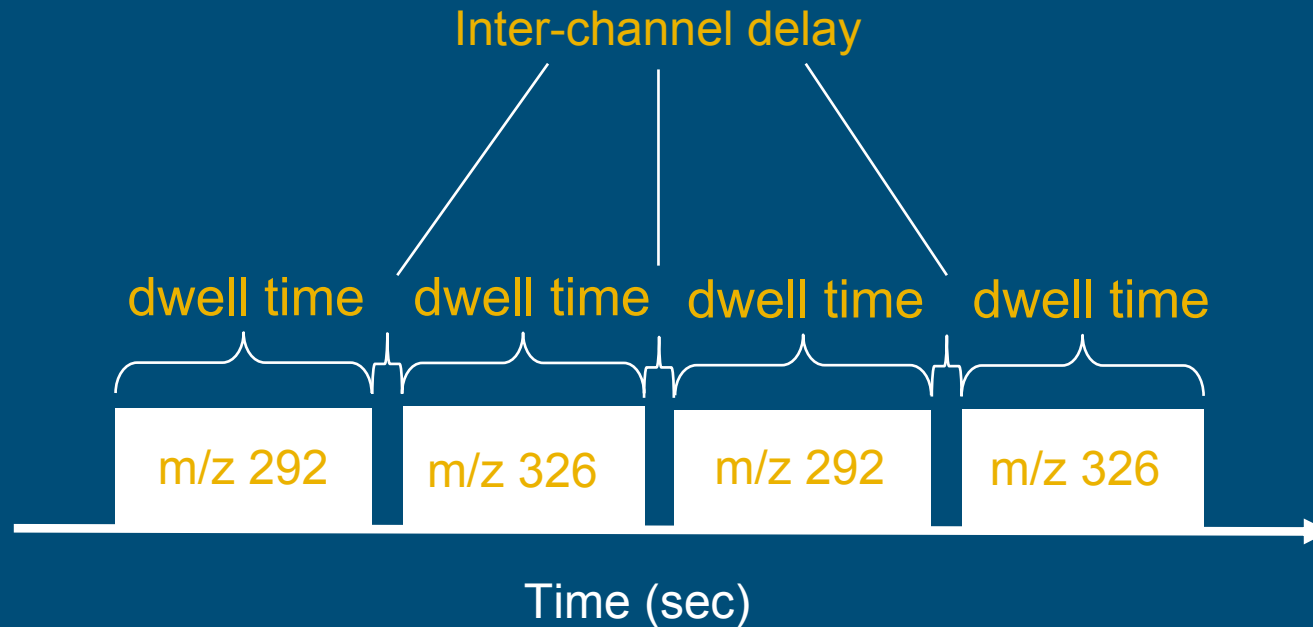
GCxGC-NCI MS chromatogram of polychlorinated alkanes



GCxGC-NCI MS chromatogram of polychlorinated alkanes



Data acquisition rate in SIR mode



$$\text{Data acquisition rate (Hz)} = \frac{1}{\sum_{i=1}^n (\text{dwell time} + \text{inter-channel delay})_i}$$



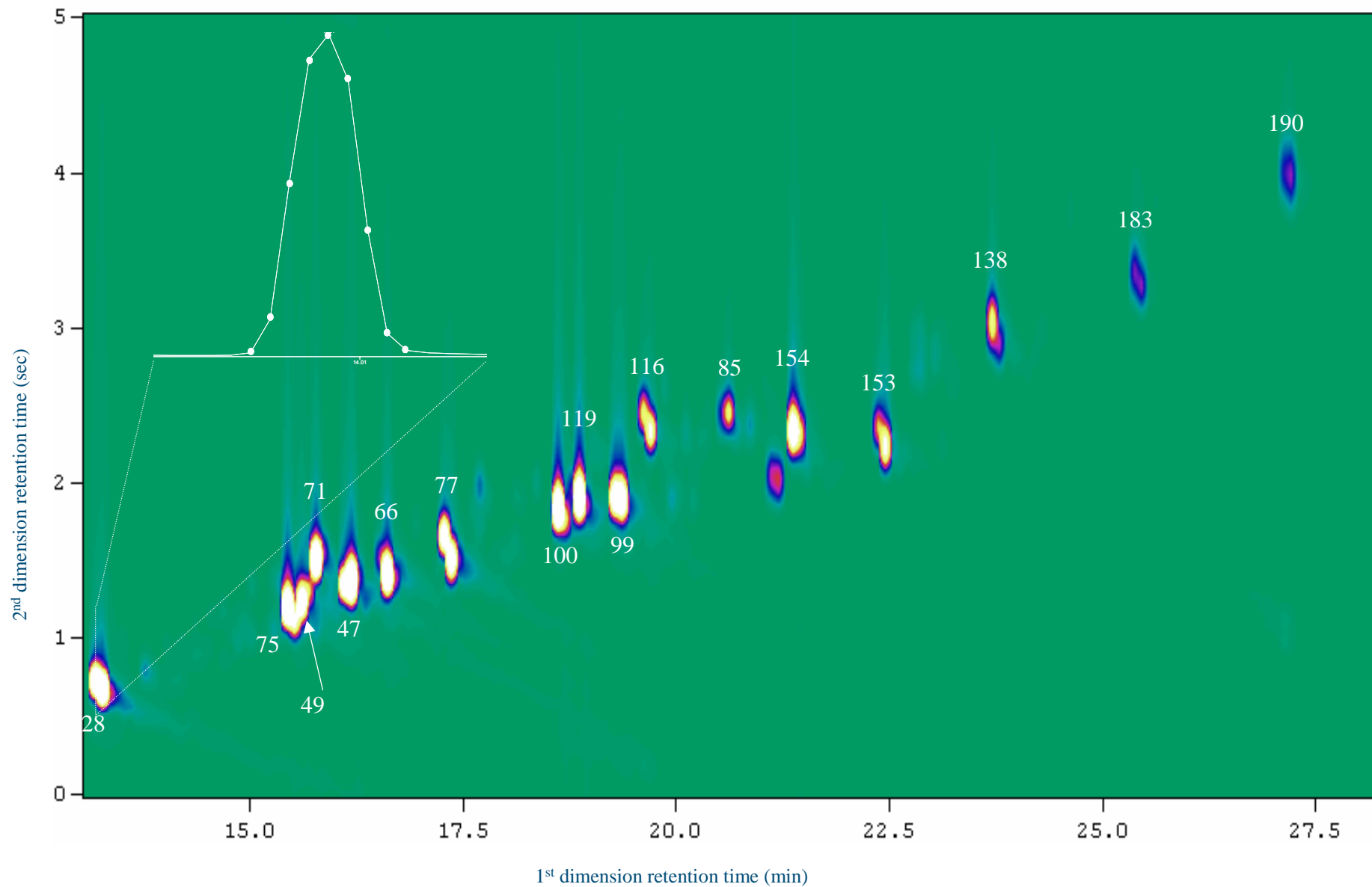
Capability of qMS in SIR mode

Number of ions	Dwell time (sec)	Inter-channel delay (sec)	Data acquisition rate (Hz)	Detectable peak width (ms)*
1	0.01	0.001	91	77
	0.02	0.001	48	146
	0.03	0.001	32	219
	0.04	0.001	24	292
2	0.01	0.001	45	156
	0.02	0.001	24	292
3	0.01	0.001	30	233
4	0.01	0.001	23	304

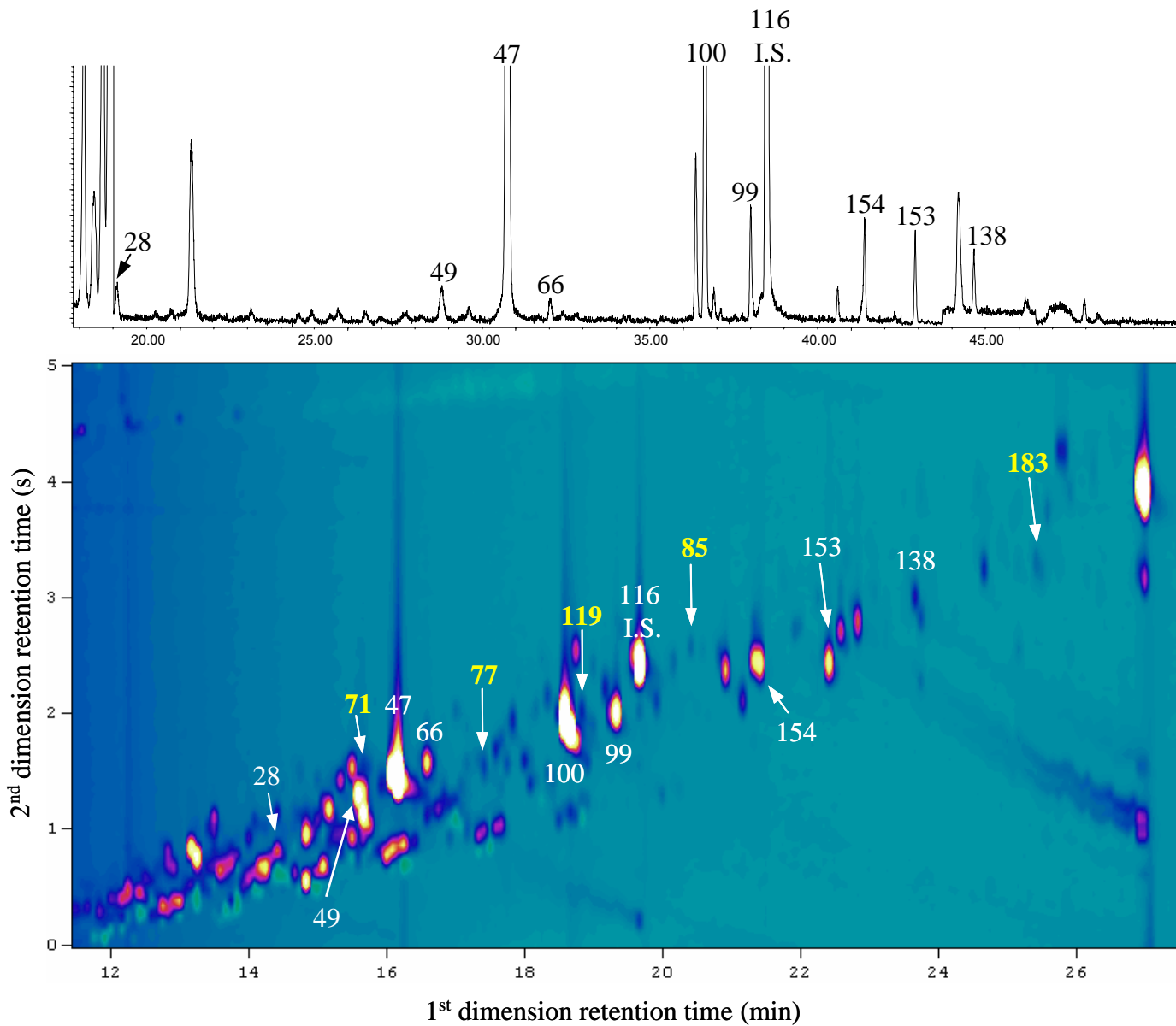
* calculated for 7 points per peak



GC×GC–SIR NCI MS chromatogram of BDEs



GC×GC–SIR NCI MS chromatogram of eel BDE extract



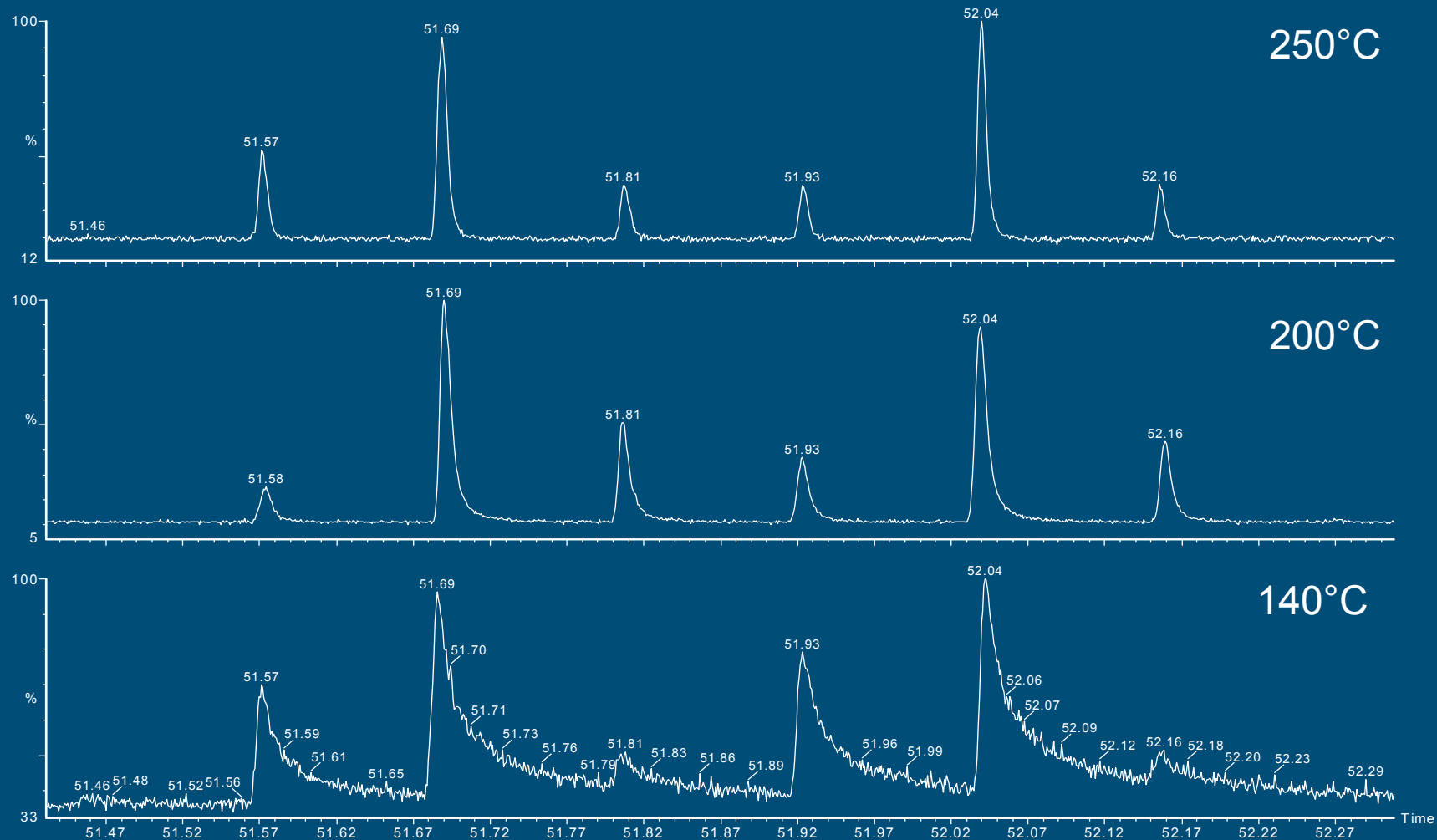
Limits of detection for selected BDEs

BDE	LOD [fg]	BDE	LOD [fg]
71	10	154	15
47	10	153	30
100	10	138	20
119	10	183	40
85	20	190	150

Monitored ions 79 and 81, dwell time 0.02 sec, source temperature 200°C



Optimization of source temperature for PCDD/Fs



Limits of detection for PCDD/Fs

Compound	Ions monitored	LODs [fg]
2,3,7,8-TCDD	[M] ⁻ 320+322	710
1,2,3,7,8-PeCDD	[M] ⁻ 354+356	40
1,2,3,4,7,8-HxCDD	[M-Cl] ⁻ 355+353	30
1,2,3,6,7,8-HxCDD	[M] ⁻ 390+392	20
1,2,3,7,8,9-HxCDD	[M-Cl] ⁻ 355+353	50
1,2,3,4,6,7,8,-HpCDD	[M-Cl] ⁻ 389+391	70
OCDD	[M-Cl] ⁻ 423+425	430
2,3,7,8-TCDF	[M] ⁻ 304+306	100
1,2,3,7,8-PeCDF	[M] ⁻ 338+340	30
2,3,4,7,8-PeCDF	[M] ⁻ 338+340	10
1,2,3,4,7,8-HxCDF	[M] ⁻ 374+376	10
1,2,3,6,7,8-HxCDF	[M] ⁻ 374+376	10
1,2,3,7,8,9-HxCDF	[M] ⁻ 374+376	10
2,3,4,6,7,8-HxCDF	[M] ⁻ 374+376	100
1,2,3,4,6,7,8-HpCDF	[M] ⁻ 408+410	10
1,2,3,4,7,8,9-HpCDF	[M] ⁻ 408+410	50
OCDF	[M] ⁻ 442+444	110



Conclusions

- Fast scanning quadrupole MS is suitable for GC×GC
- Mass range of 300 Da can be acquired at data acquisition rate of 23 Hz
- Data acquisition rate in SIR mode can be up to 91 Hz, if only one ion is monitored
- Excellent technique for studying the elution characteristic of polychlorinated alkanes
- LODs for BDE congeners are from 10 to 150 fg
- LODs for PCDD/Fs are from 10 to 700 fg

