PEFTEC PETROLEUM & REFINING TECHNOLOGIES
VIRTUAL EVENT 24TH & 25TH NOVEMBER 2021

Short course-GC×GC: Day 1
- Fundamentals of GC×GC

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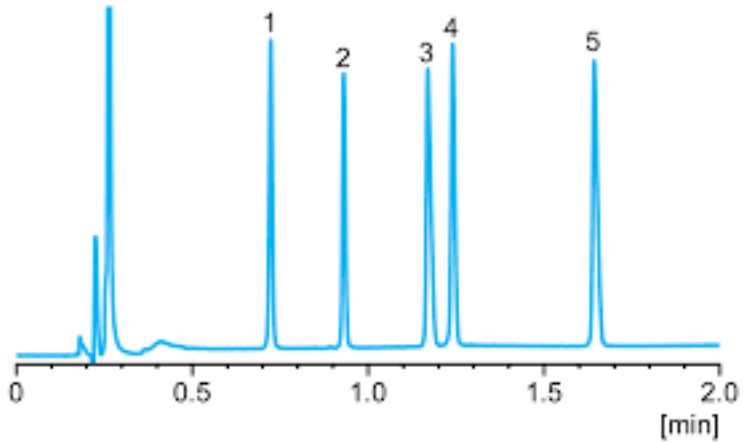
LIÈGE université
MolSys

Chromatography: A physical method of separation in which the components to be separated are distributed between two phases, one of which is stationary (stationary phase) while the other (the mobile phase) moves in a definite direction.

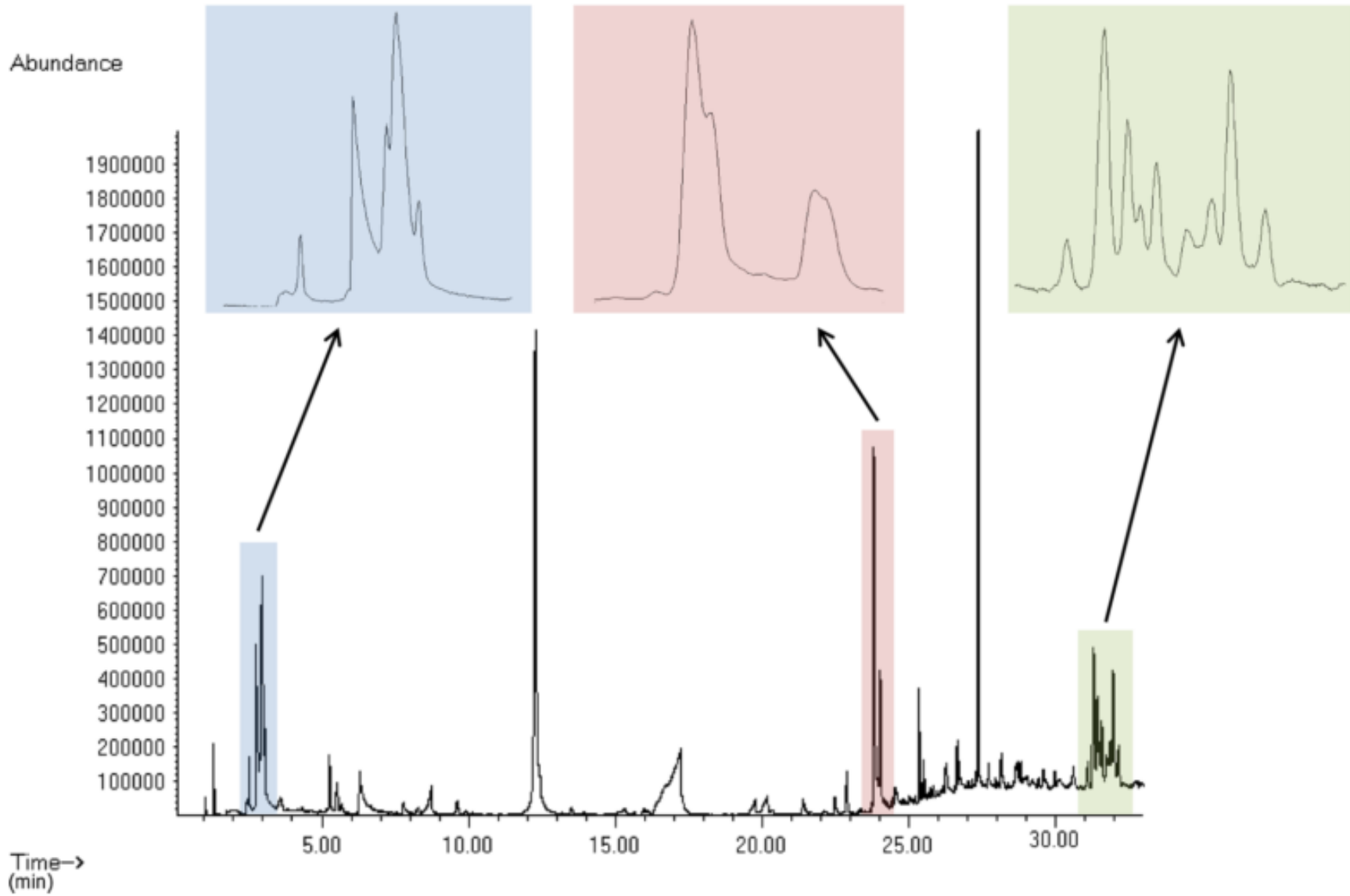
IUPAC Gold Book



The sample

The sample

Abbey


Abundance
1900000
1800000
1700000
1600000
1500000
1400000
1300000
1200000
1100000
1000000
900000
800000
700000
600000
500000
400000
300000
200000
100000
5.00
10.00
15.00
20.00
25.00
30.00
Time→
(min)

Abbey

Abbey

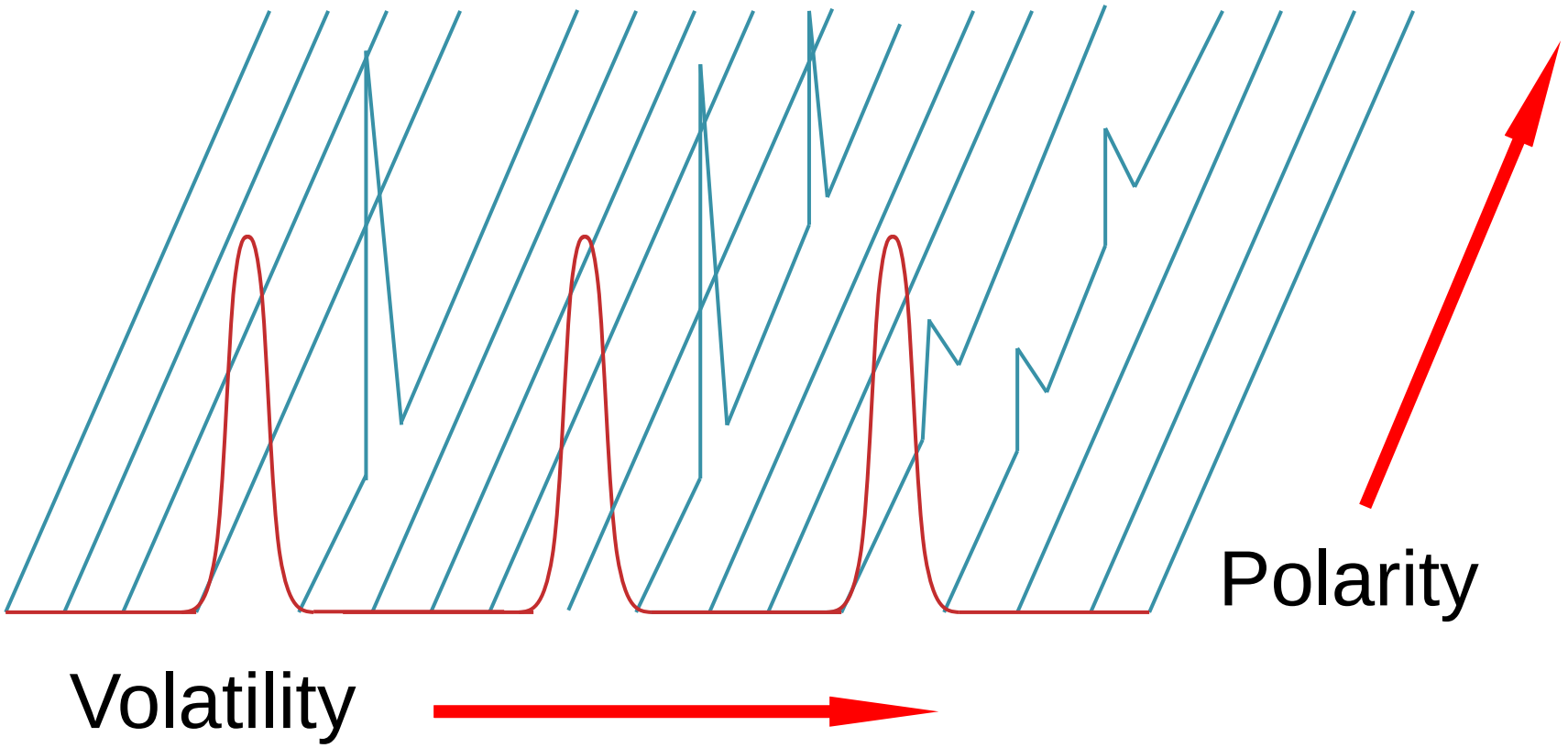
Limitations:

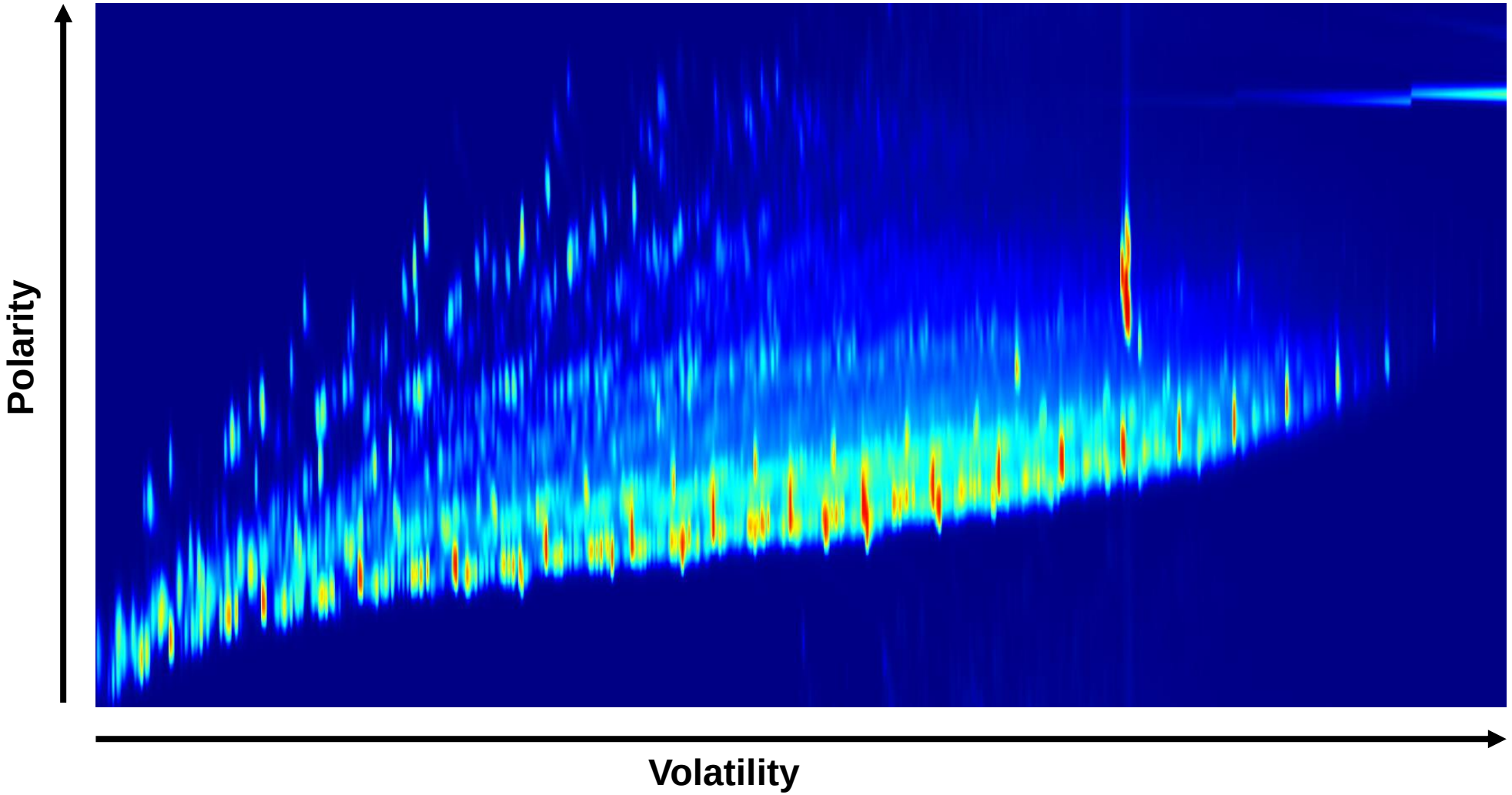
- Peak broadening
- Run duration
- …

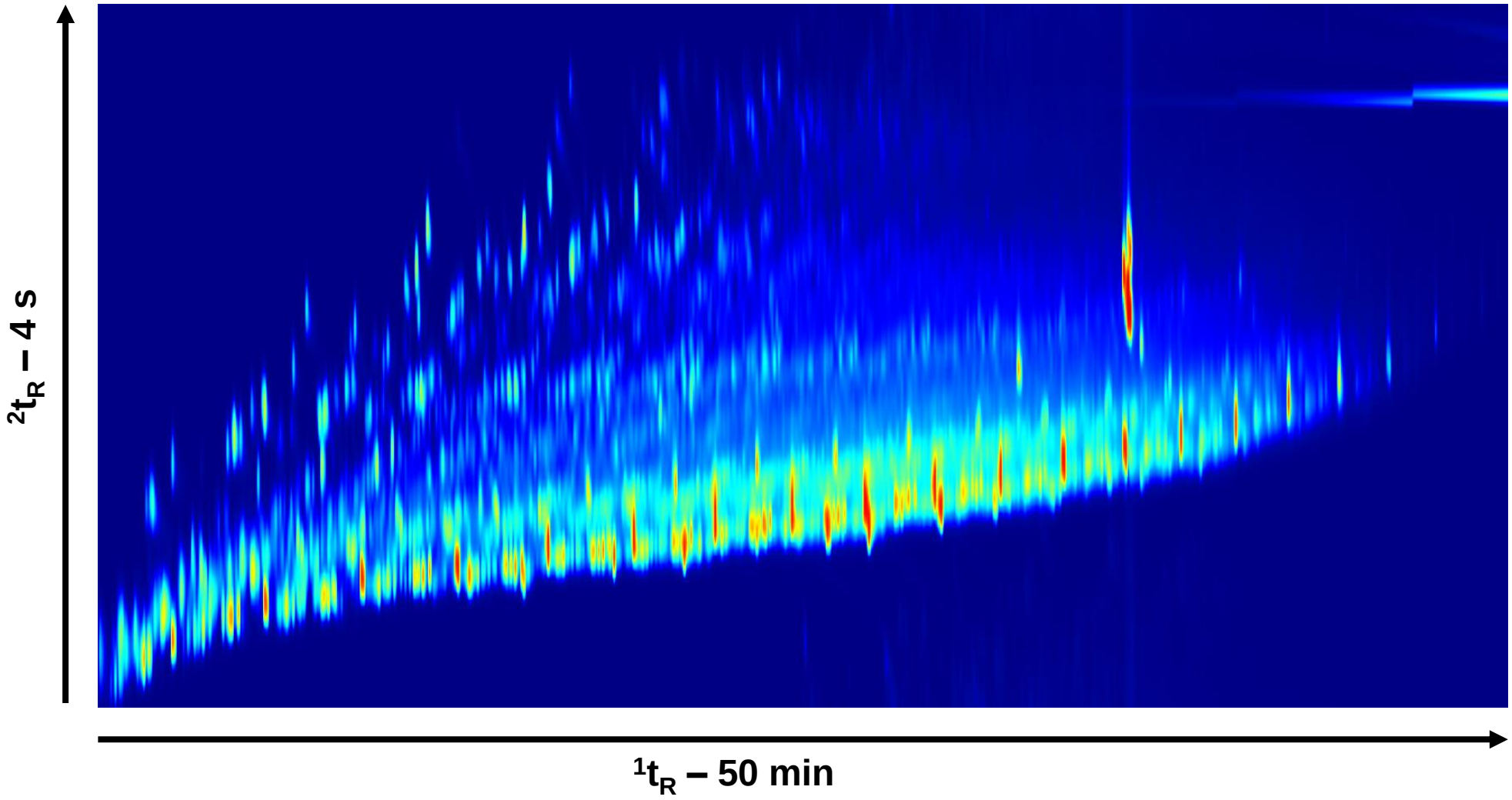
Adding an extra dimension

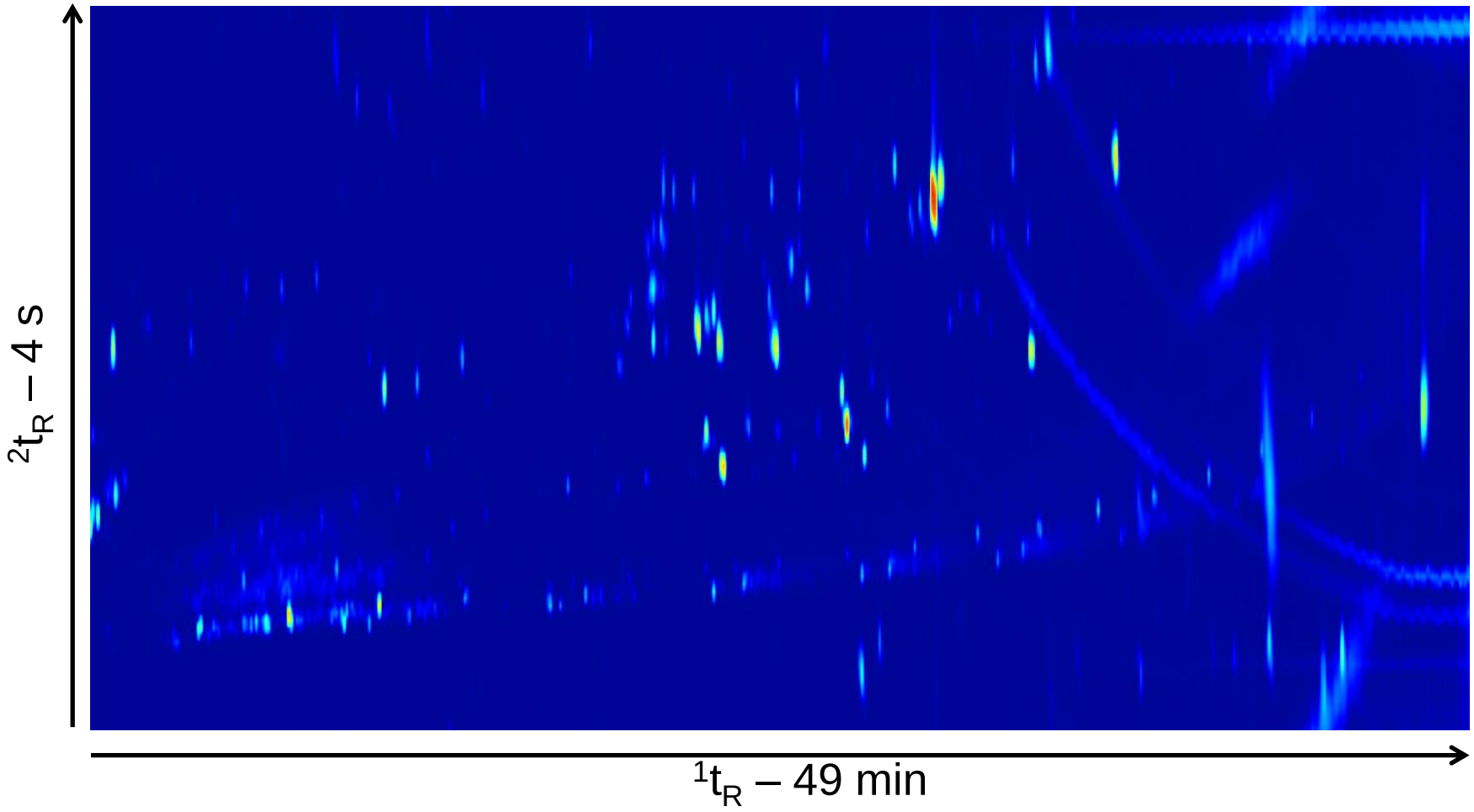

Beer Type
Abbey


Abbey
Beer Color
PUUR
CHIMAY
CHIMAY
CHIMAY

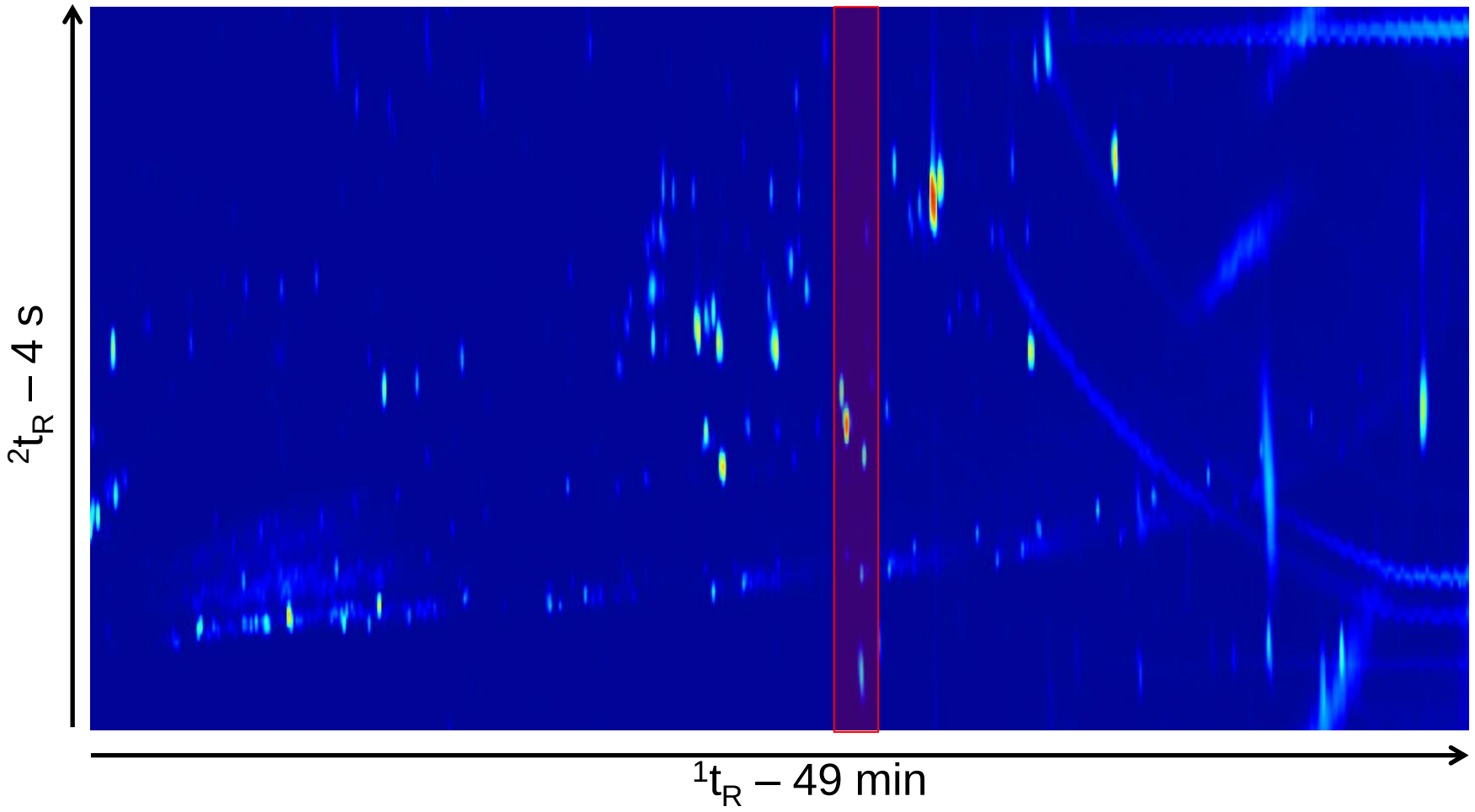

Polarity
Volatility


Polarity
Volatility


^2t_R – 4 s
^1t_R – 50 min

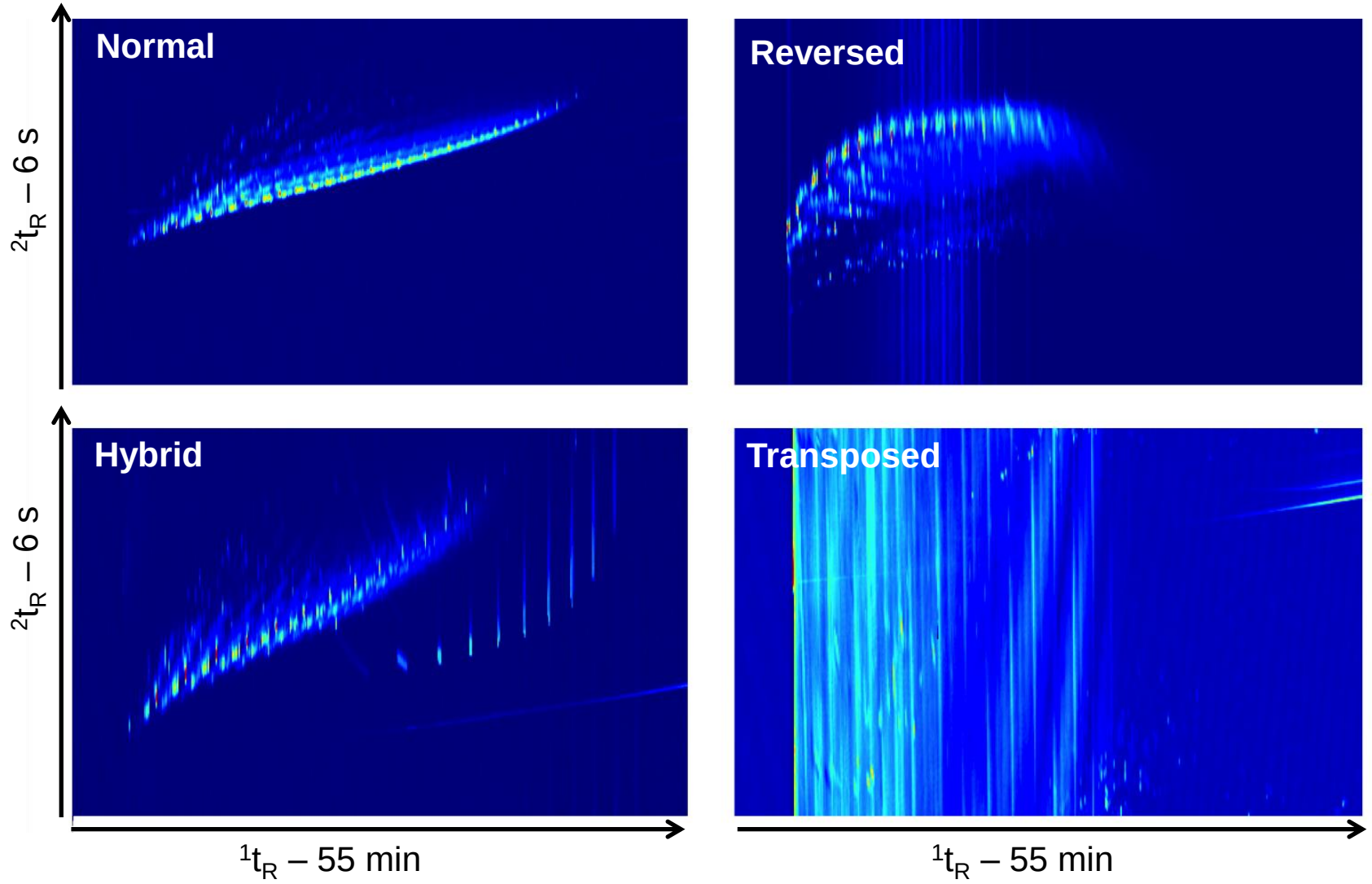

$^{2}t_R$ – 4 s
$^{1}t_R$ – 49 min

5



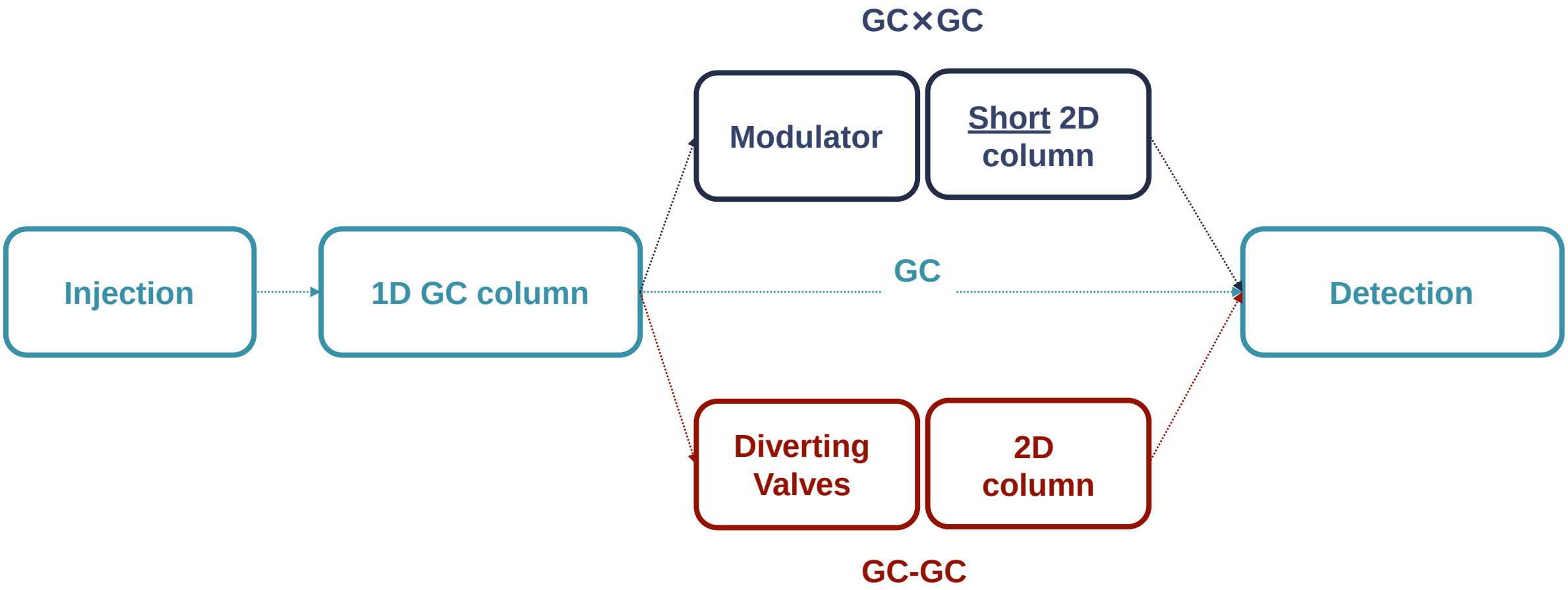
2.4333
1.9333
1.4333
2036
2236
2436

GC×GC separation classification

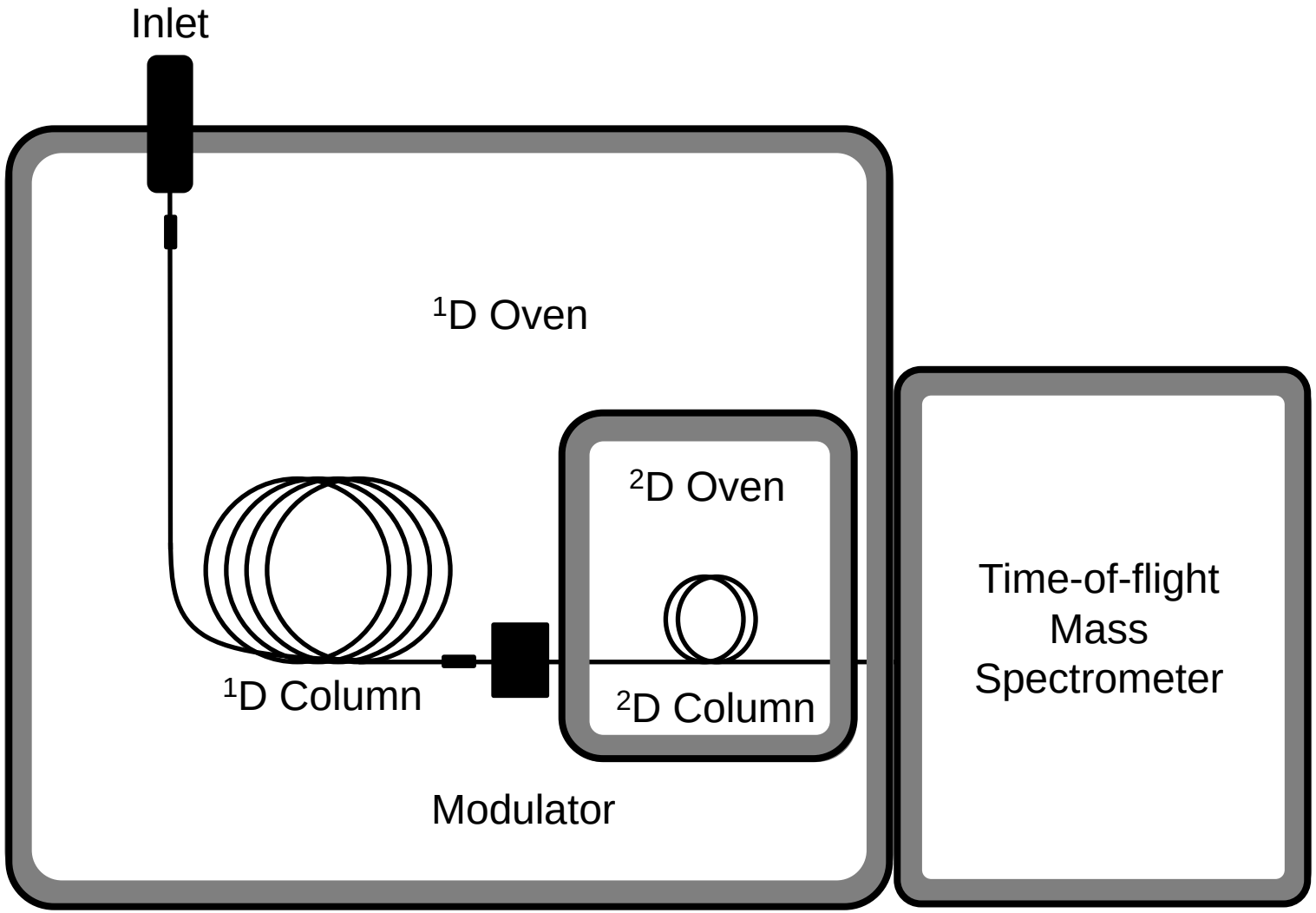


The “comprehensive” hardware

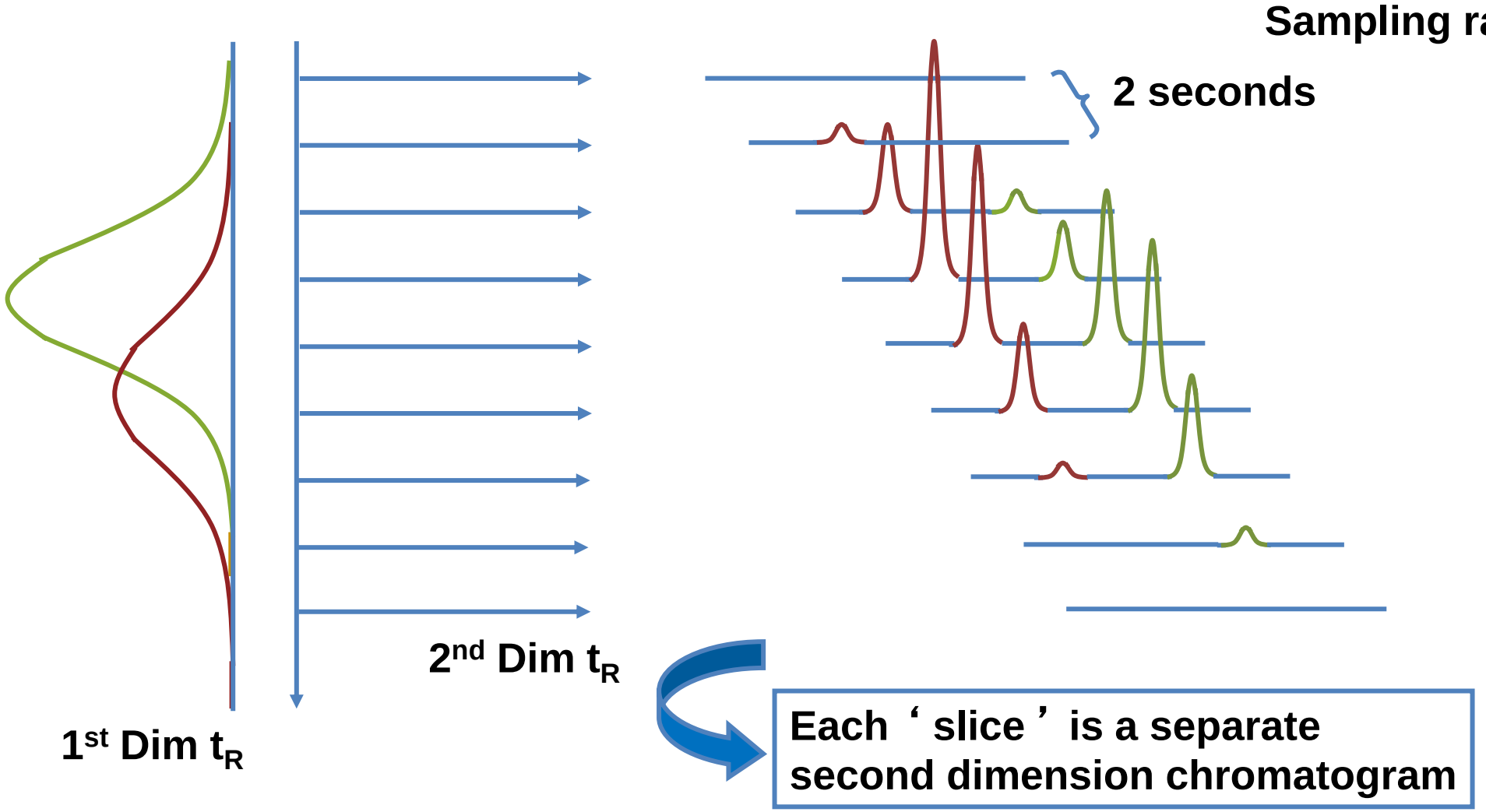
GC×GC: How does it work?



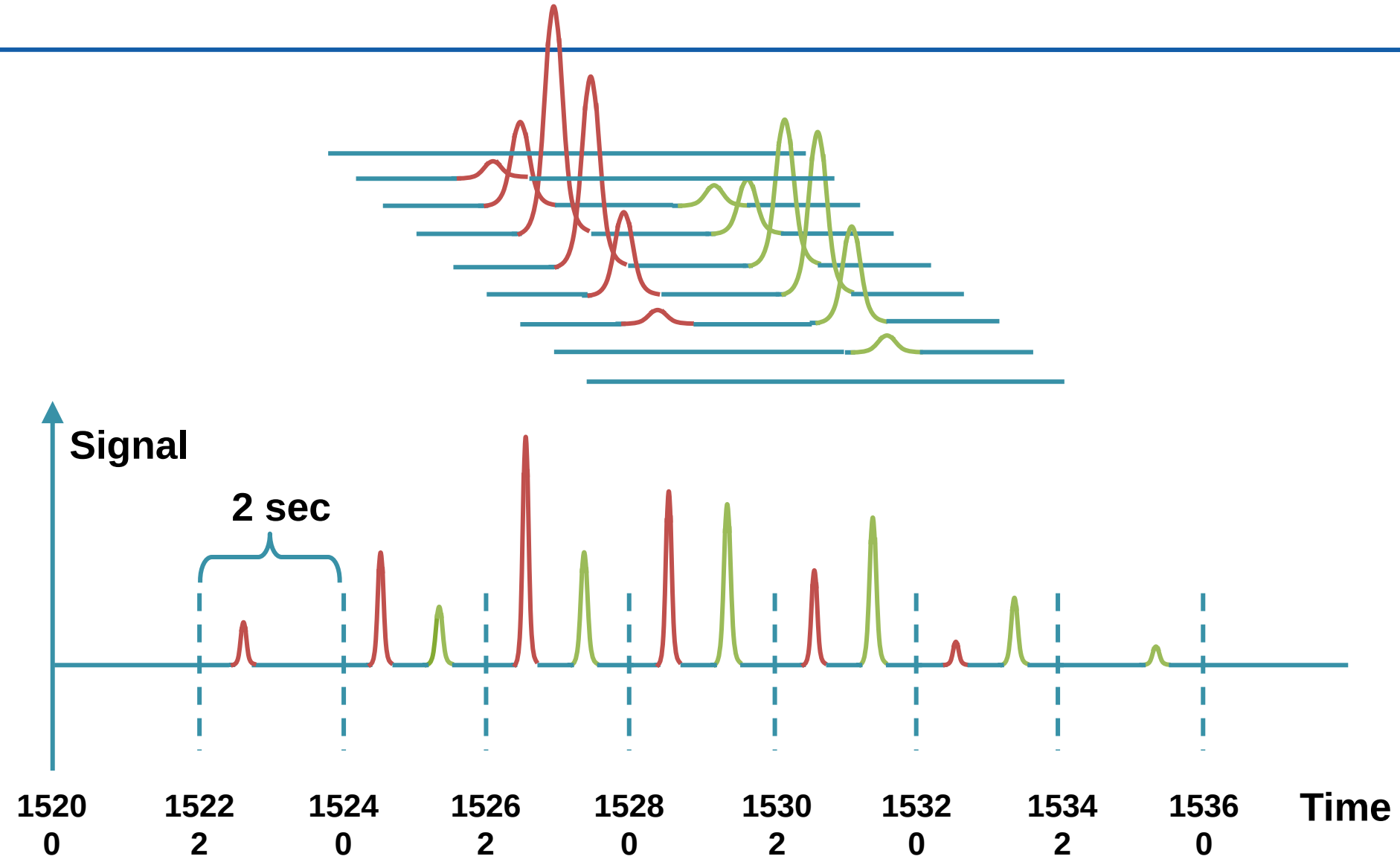
GC×GC: How does it work?



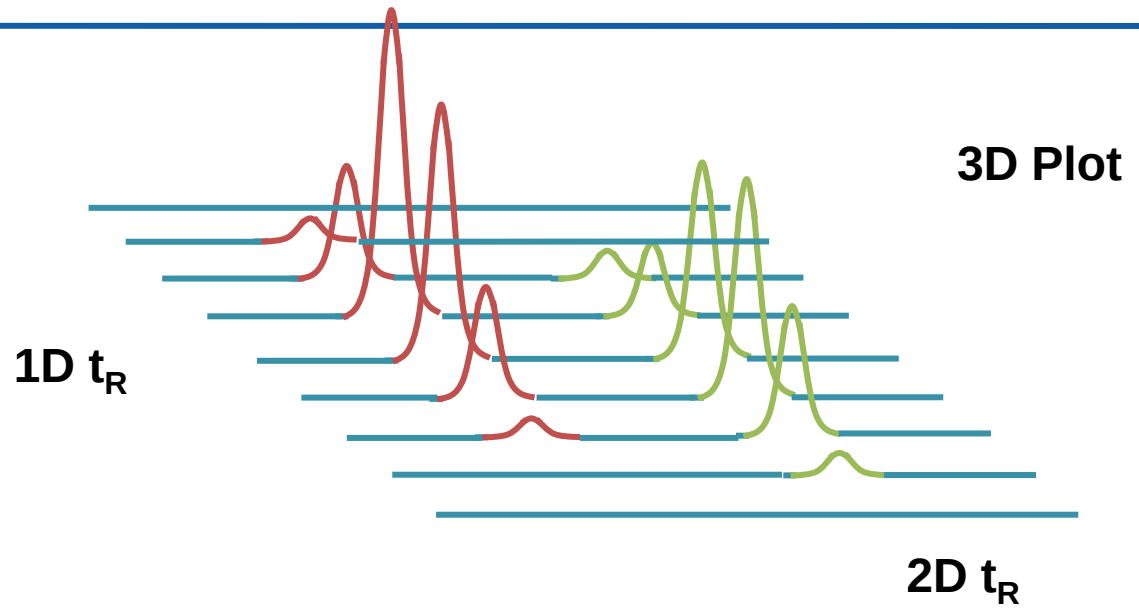
Modulation Process



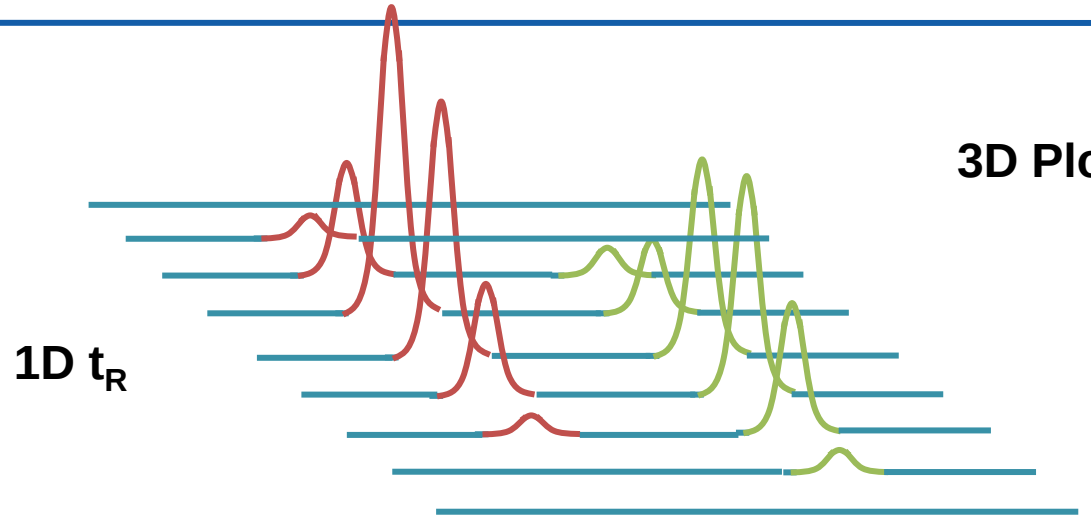
Signal at the detector

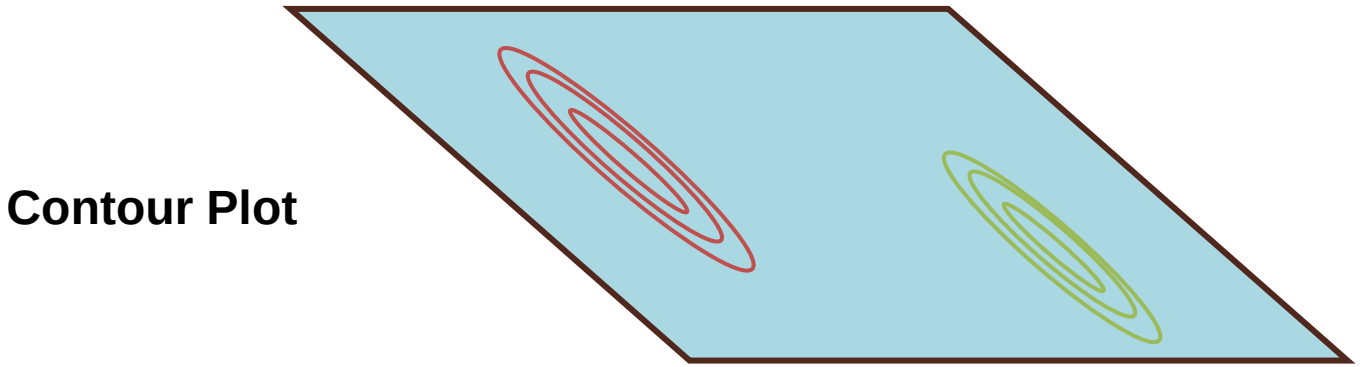


Signal Display



Signal Display

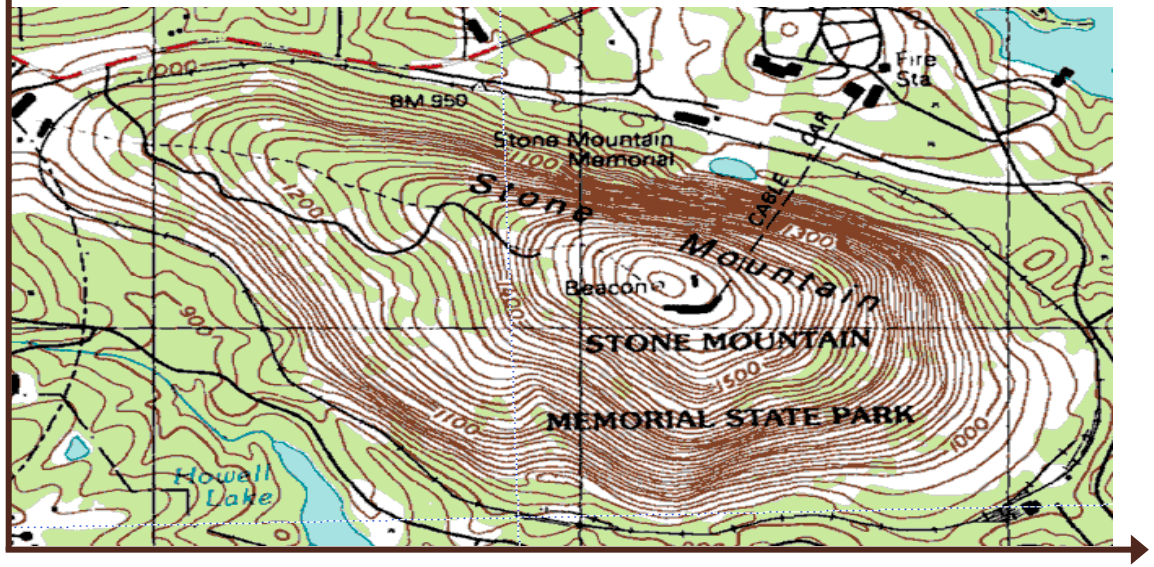




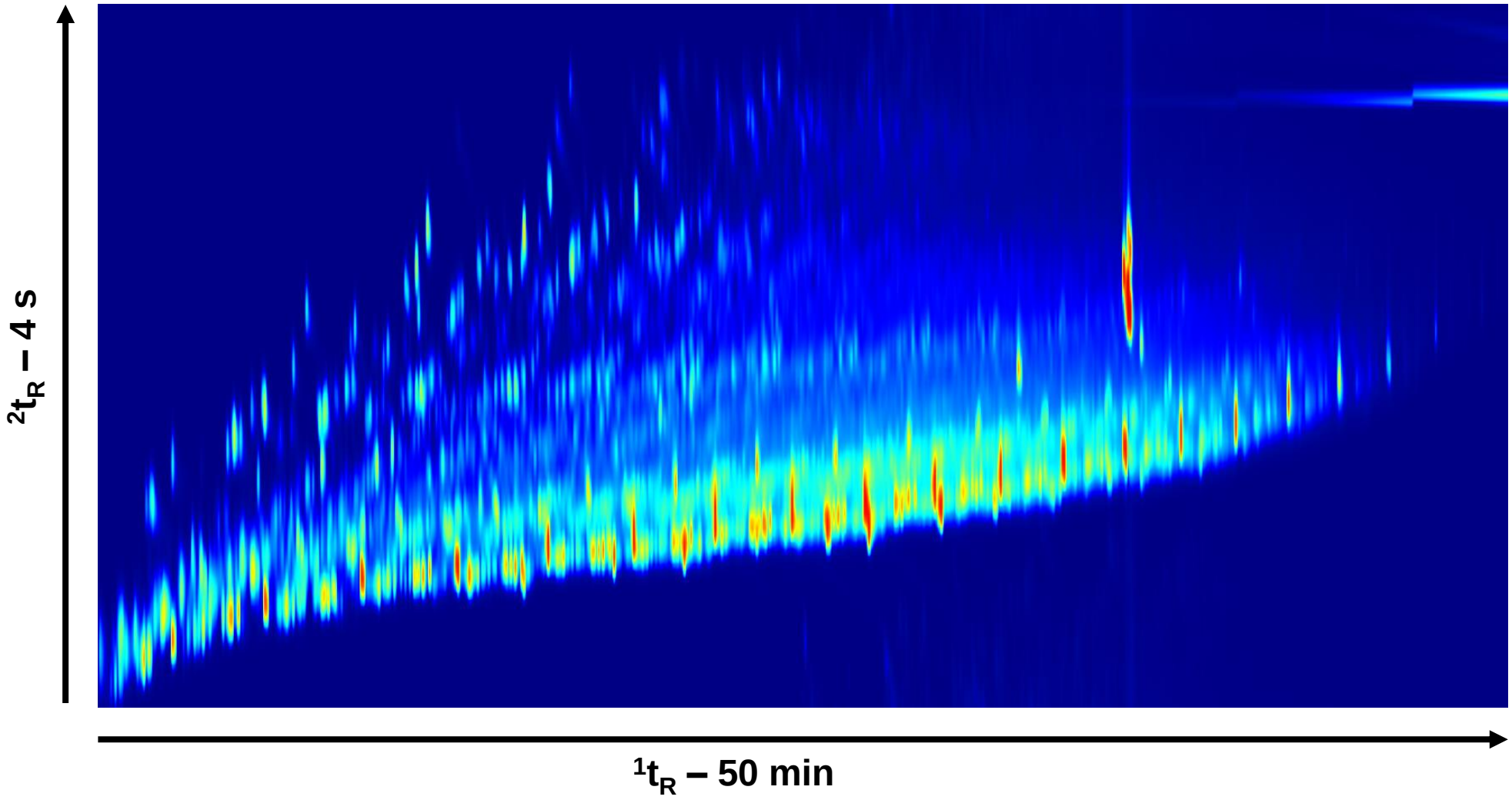
1st Dim t_R

2nd Dim t_R

1st Dim t_R

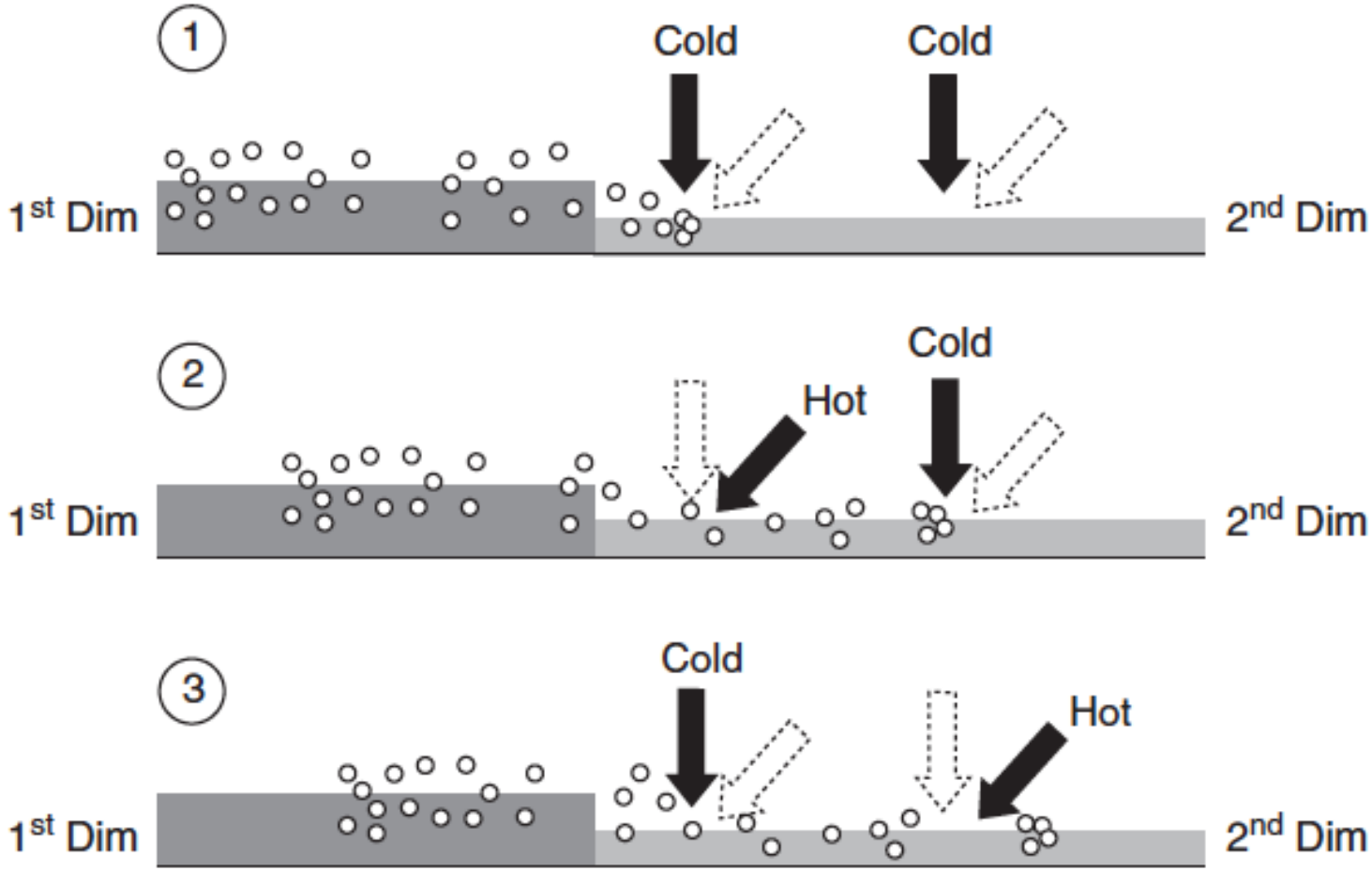


2nd Dim t_R

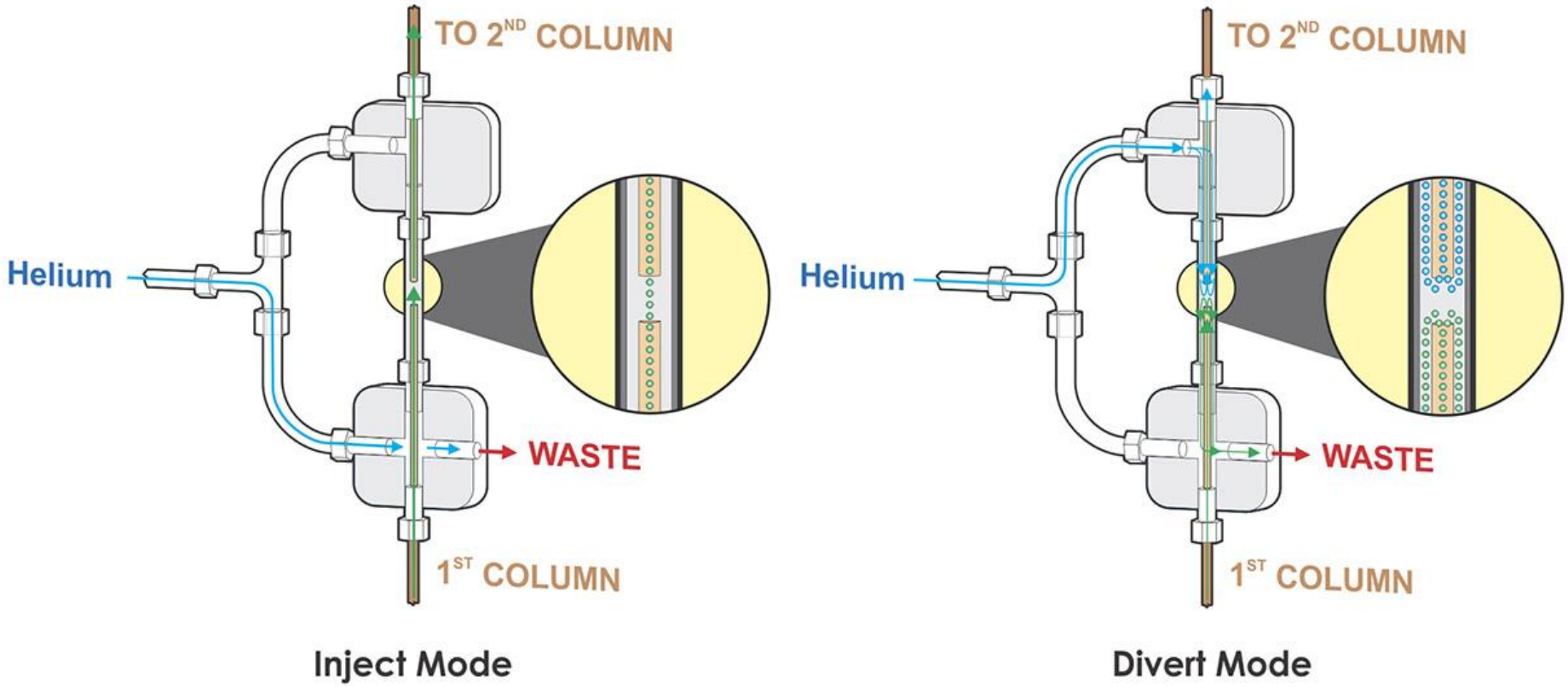

^2t_R – 4 s
^1t_R – 50 min

The “comprehensive” hardware

Cryogenic Modulator

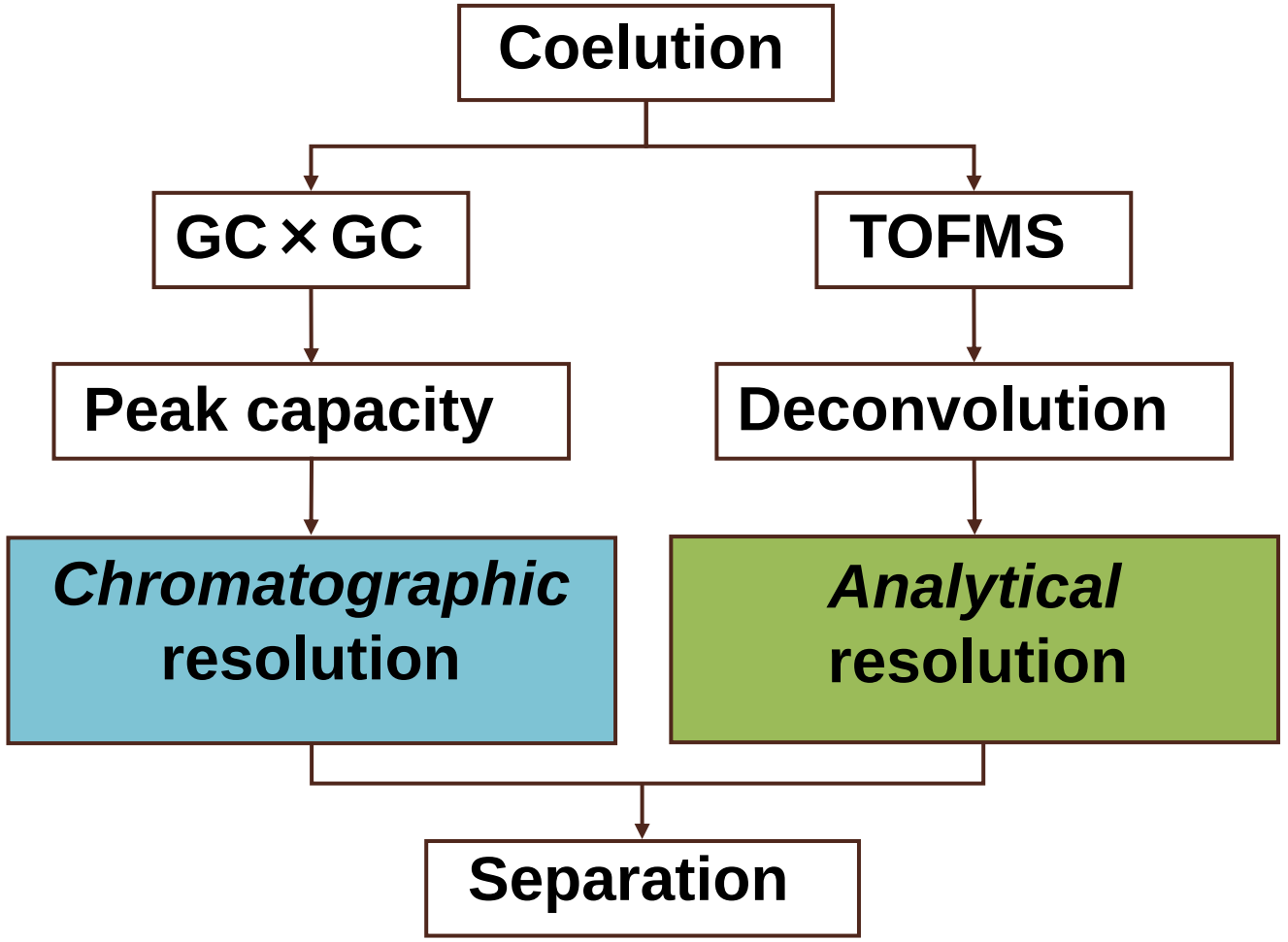


Flow Modulator

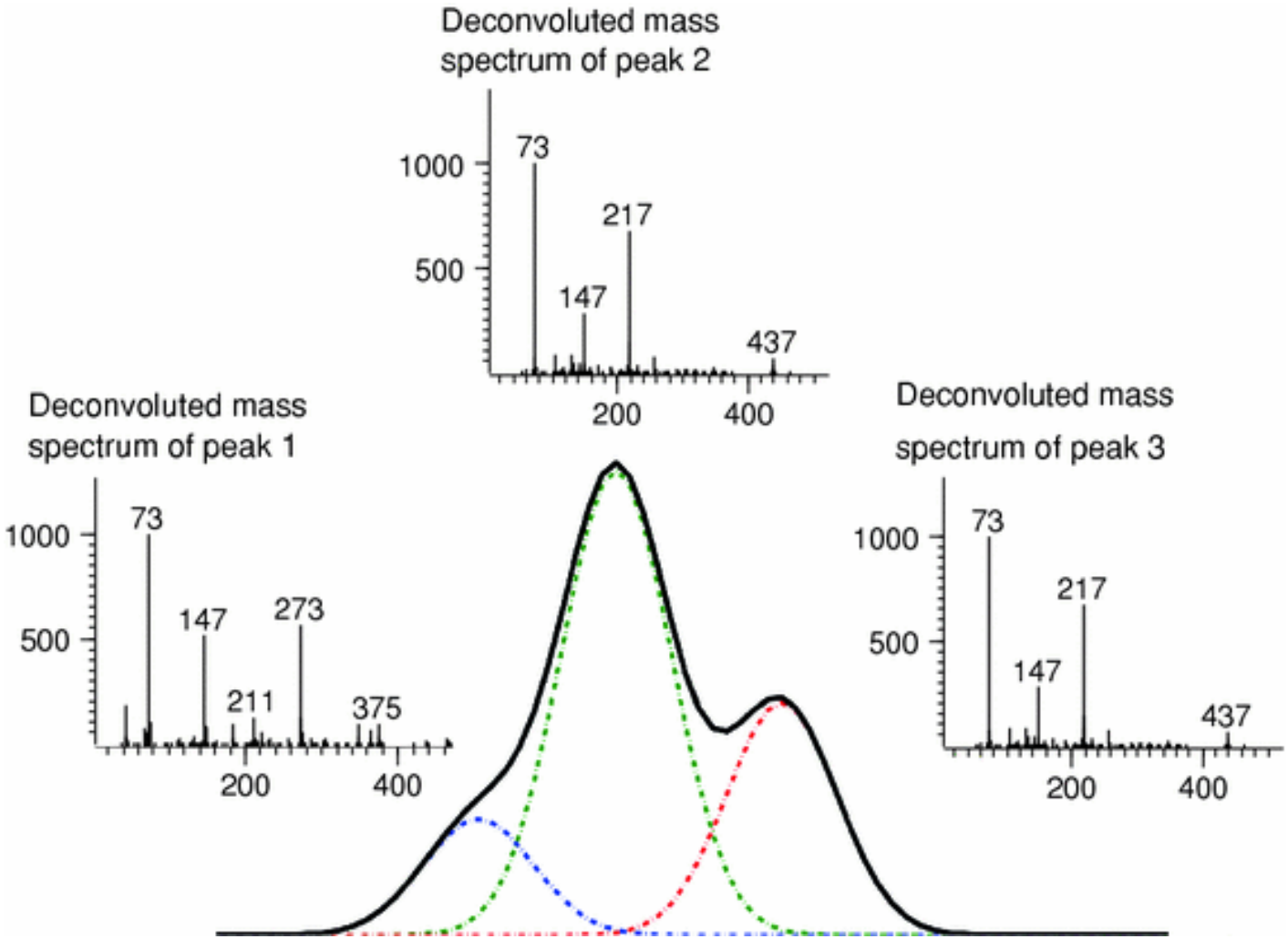


Adding the MS dimension

Coelution solving power



Coelution solving power



Some Good MS Tools

LRTOFMS

200 Hz

LR (unit)

-

Deconvolution

EI

-

Comprehensive

HRTOFMS

200 Hz

HR (>50,000)

Accuracy < 1ppm

Deconvolution

EI, PI, NCI,…

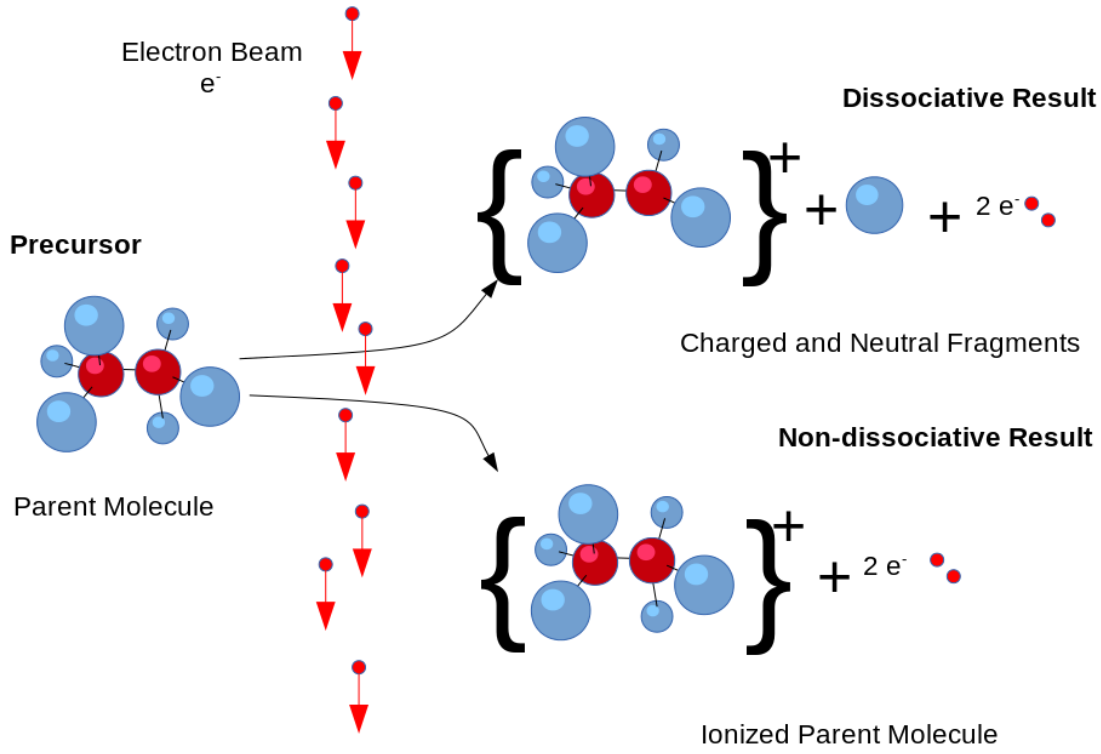
Elemental analysis

Comprehensive

Depends on the needs…

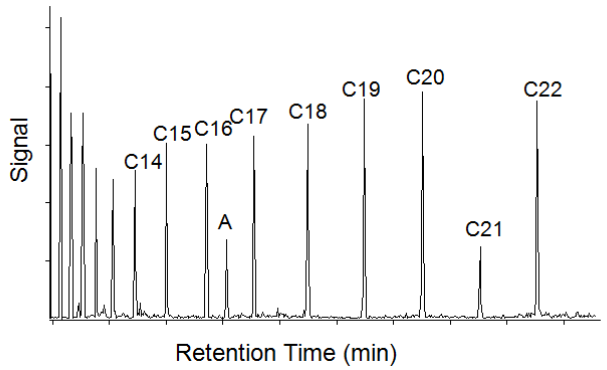
Electron ionization – 70 eV

→ **MS spectra = fingerprint of a compound**



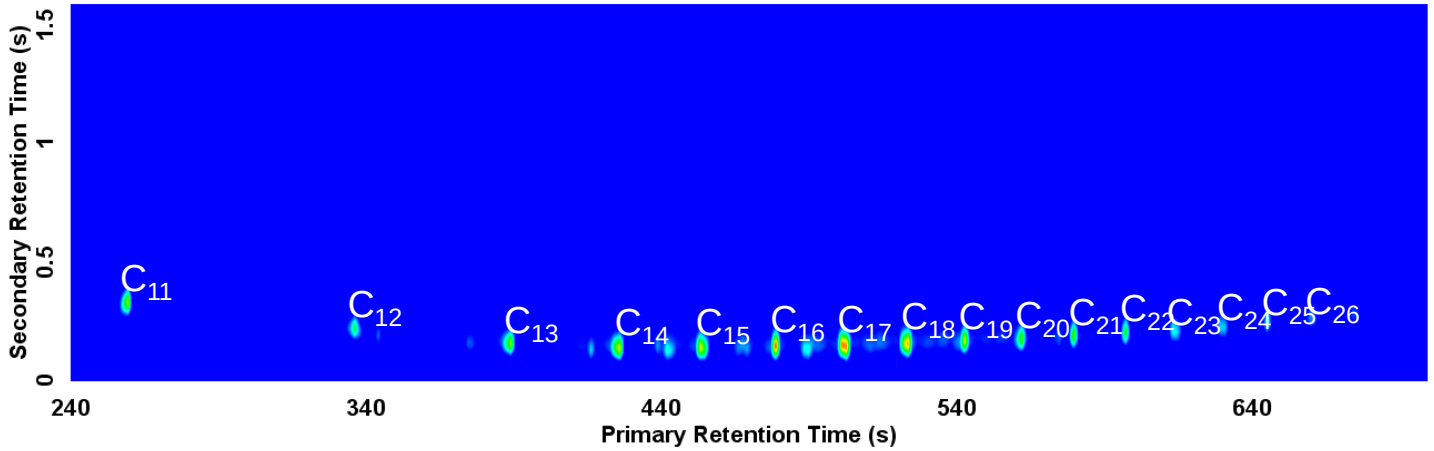
Retention Index

- Used to convert retention times to a constant that is independent from the system
- Normalization of retention time to the retention time of alkanes

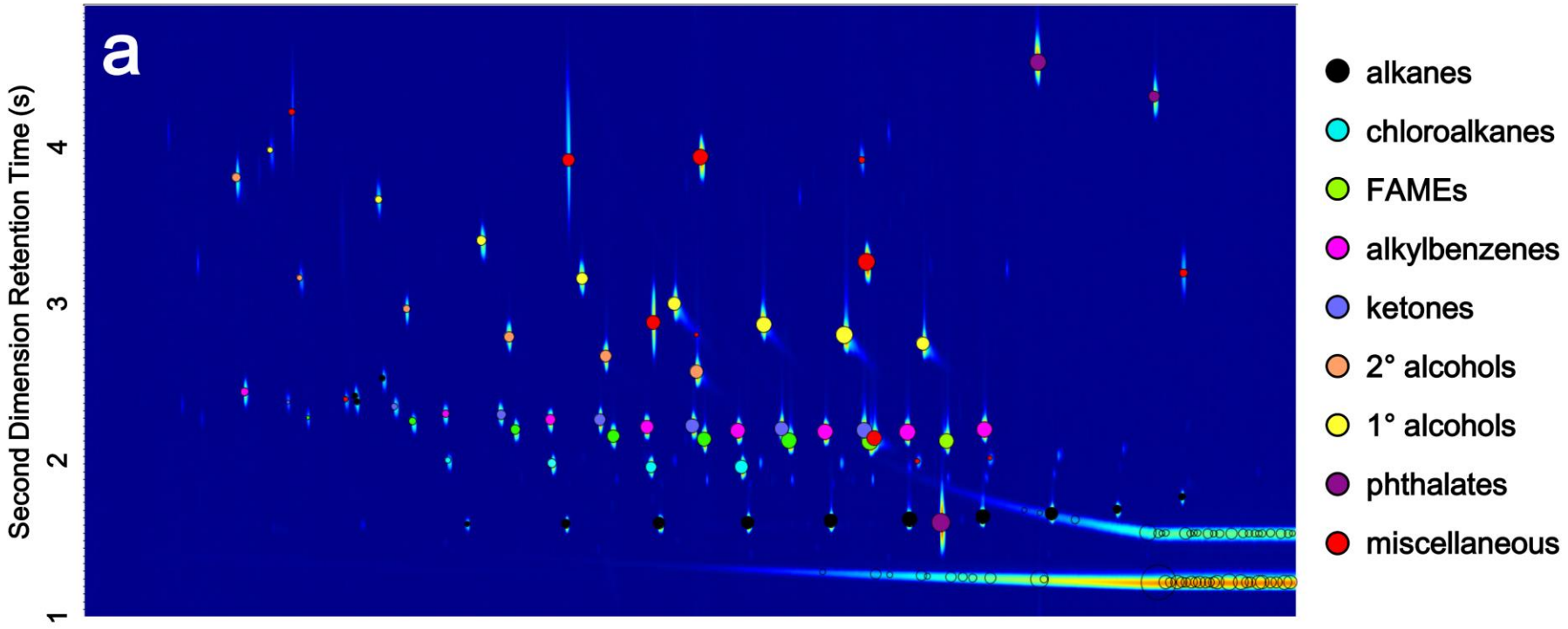


$$I = 100\left(n + \frac{t_{R(unknown)} - t_{R(n)}}{t_{R(N)} - t_{R(n)}}\right)$$

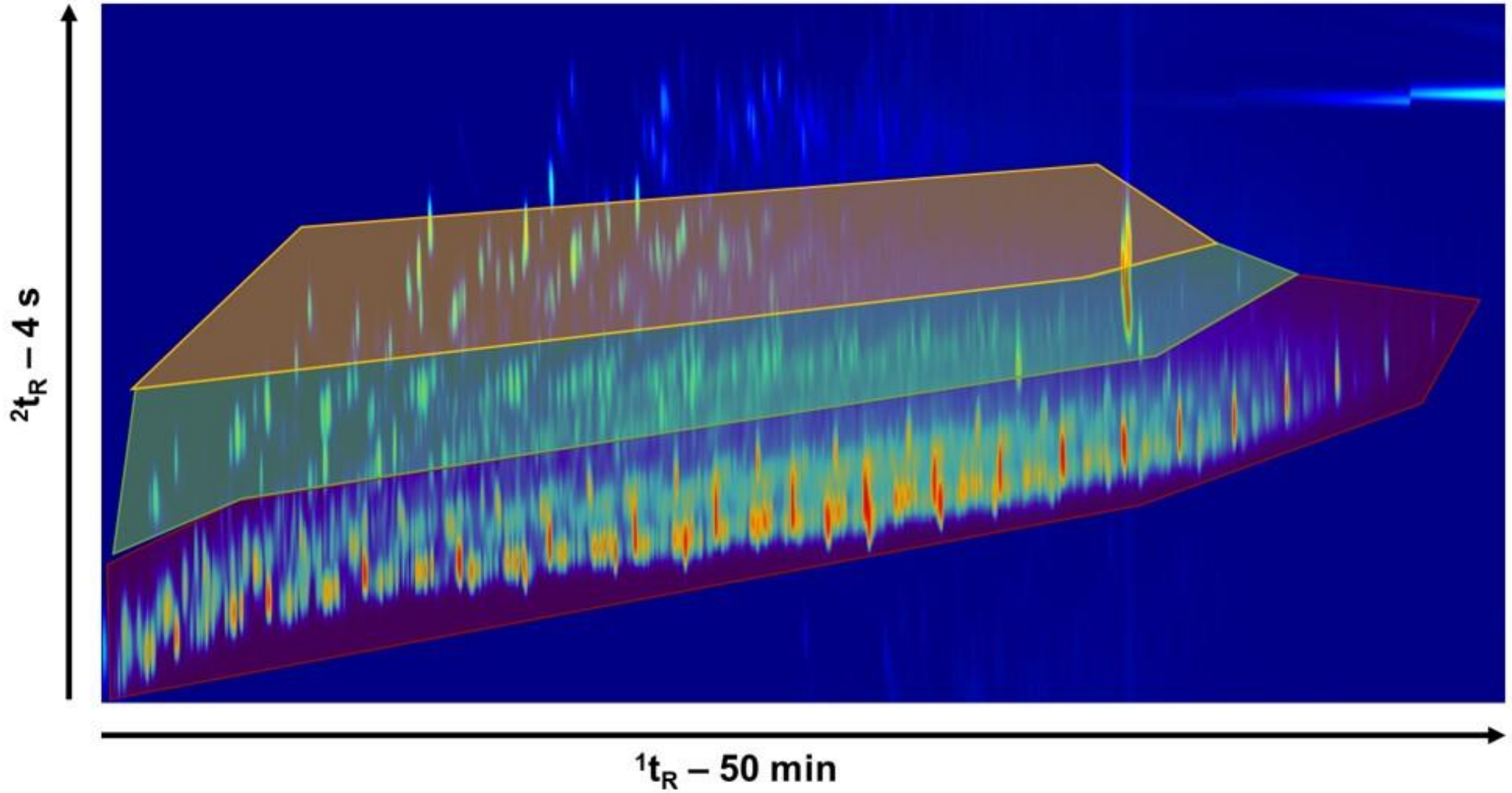
n: number of C in smaller n-alkane
N : number of C in larger n-alkane
t_R : retention time

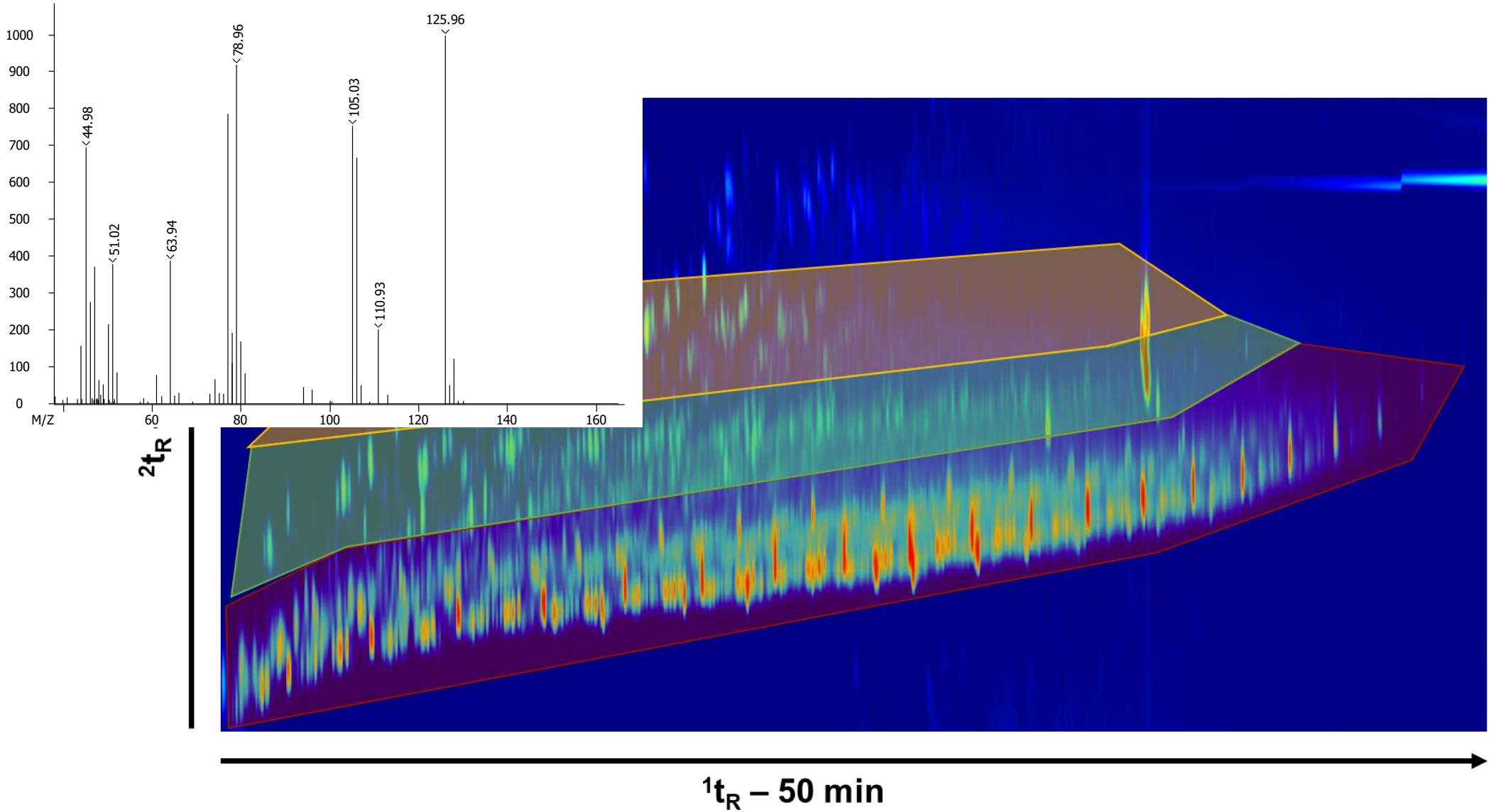


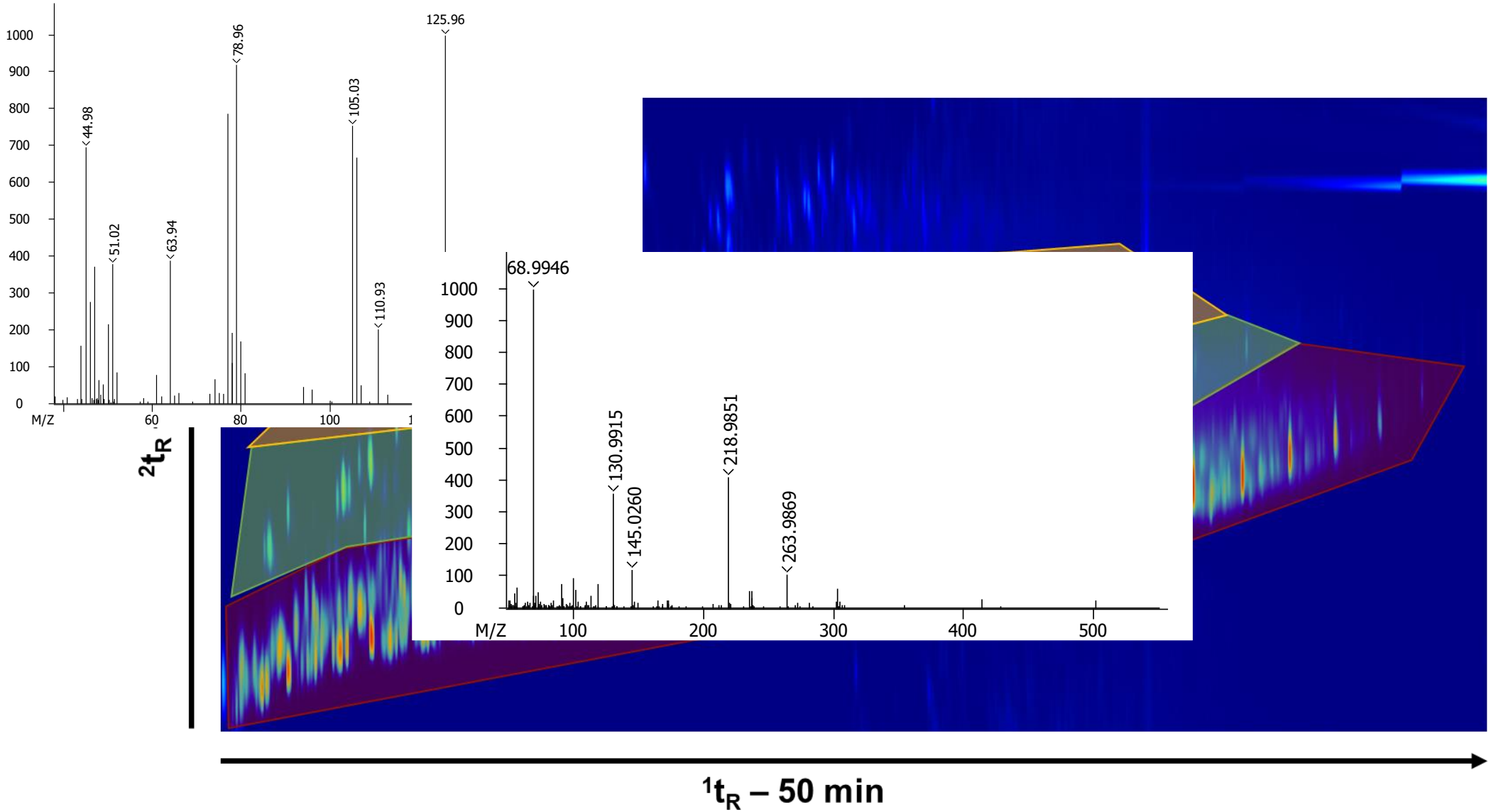
Structured 2D separation

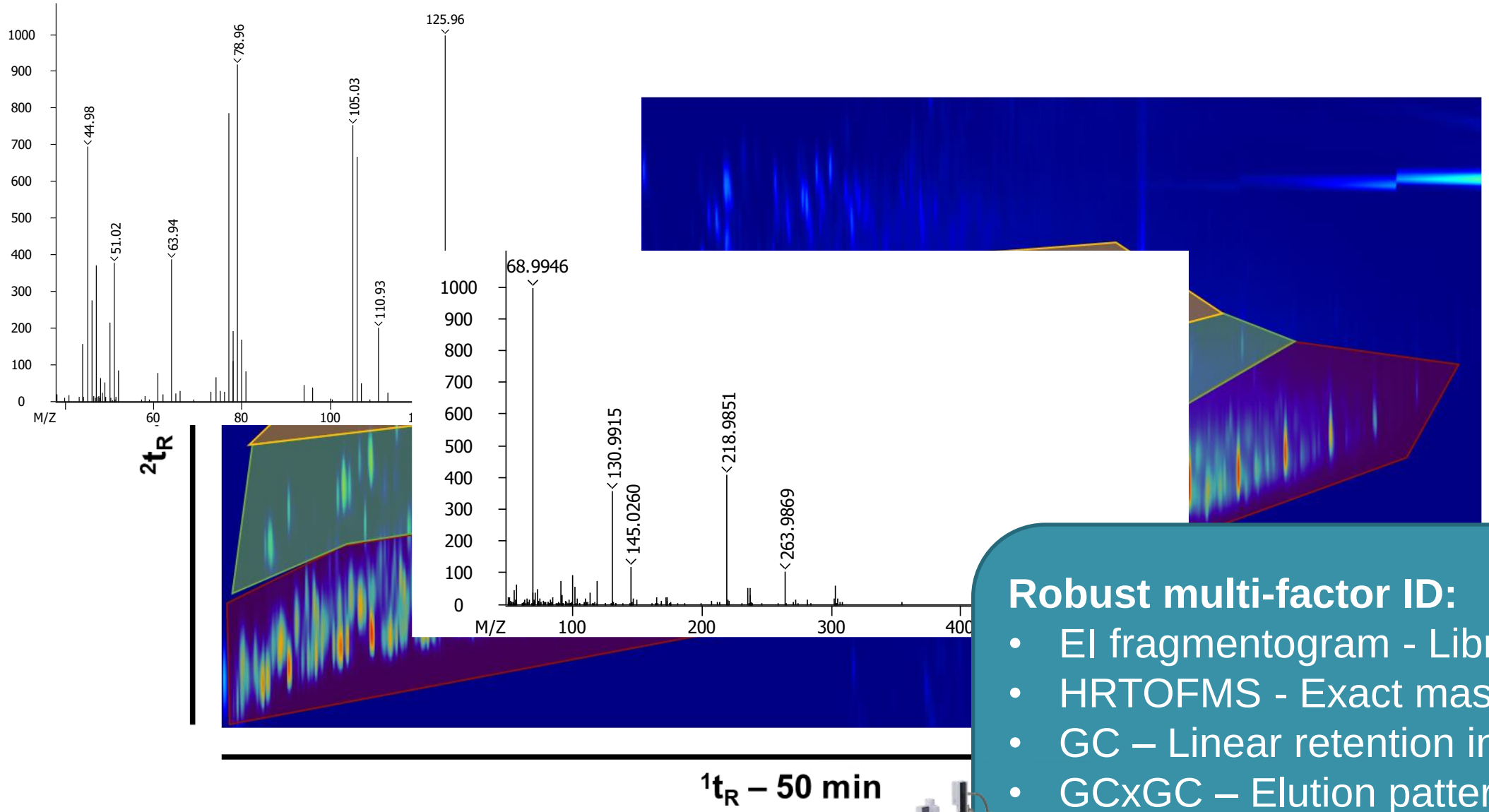


Structured 2D separation




125.96
78.96
105.03
44.98
110.93
51.02
63.94
1000
900
800
700
600
500
400
300
200
100
0
M/Z
60
80
100
120
140
160
2tR
1tR – 50 min


125.96
78.96
105.03
44.98
51.02
63.94
110.93
1000
900
800
700
600
500
400
300
200
100
0
M/Z
60
80
100
68.9946
130.9915
145.0260
218.9851
263.9869
100
200
300
400
500
2tR
1tR – 50 min



Robust multi-factor ID:

- EI fragmentogram - Library match
- HRTOFMS - Exact mass
- GC – Linear retention indices
- GCxGC – Elution pattern

→ Level 2 MSI ID