

**Molecular components map of
representative matrices of commodity
groups in Document SANTE/11813/2017**

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1. Aim and scope

This report updates the “component map” for typical representative commodities of each commodity group in Document SANTE/11945/2015.

2. Short description

“Molecular component map” was developed for new 42 commodities belonging from seven commodity groups. Egg and liver were extracted at the EURL-AO laboratory. Fish feed, oat and hay were extracted at the EURL-CF laboratory. Artichoke, Brussel sprout, white cabbage, cucumber, grapefruit, green bean, lime, mandarin, mushroom, nectarine, okra, papaya, paraguayan, peach, pear, pineapple, plum, pomegranate, pumpkin, radish, raisin, raspberry, red cabbage, Romanesco broccoli, spring onion, watermelon, zucchini, cayenne, black pepper, curcuma, olive oil, sunflower oil, soya oil, hazelnuts and chia seeds were extracted at the EURL-FV laboratory; all were analysed by LC-TOF-MS at the EURL-FV laboratory. Matrix samples were injected by triplicate. Final matrix concentration was 0.2 g sample/ml for all matrices, except for chia seeds and species (0.04 g sample/ml), liver, egg and oat (0.5 g sample/ml), hay and fish feed (0.1 g sample/ml). Matrix compounds were retrieved and counted using the Molecular Feature Extractor (MFE) algorithm in the MassHunter Workstation Software. The MFE creates a compound list of all the peaks in the data file that represent real molecules. At the end of the data process, a list with the mass, retention time, and intensity of all matrix components was obtained. The resulting data was evaluated to get information on the complexity of the matrices through the number and distribution of the matrix components.

3. Procedure

3.1. Sample extraction

The buffer citrate QuEChERS method was applied to the selected matrices. The buffer citrate QuEChERS method including a sorbent for fatty matrices was applied to egg, liver, hazelnuts, chia seeds, oils and fish feed. For oat and hay, four clean-ups procedures were evaluated:

- Oat matrix (1 ml of extract)

Procedure 1	Procedure 2	Procedure 3	Procedure 4
PSA according to EN 15662 25mg/ml extract	PSA 150mg/ml extract	PSA 150 mg/ml Z-sep 150 mg/ml EMR-lipid	Z-sep 150 mg/ml EMR-lipid

- Hay matrix (6 ml extract)

Procedure 1	Procedure 2	Procedure 3	Procedure 4
150 mg Supelclean PSA, 900 mg MgSO4	150 mg Supelclean PSA, 15 mg Supelclean ENVI-Carb, 900 mg MgSO4	150 mg Supelclean PSA, 45 mg Supelclean ENVI-Carb, 900 mg MgSO4	480 mg Z-sep+ 400 mg Supelclean PSA 80 mg Supelclean ENVI-Carb, 900 mg MgSO4

3.2. Instrumentation and analytical conditions for the LC-TOF-MS

3.2.1. Agilent 1290 HPLC

- Column: Agilent Eclipse Plus Rapid Resolution HD C18, 2.1 mm x 50 mm x1.8 µm
- Mobile phase A: Methanol 0.1% Formic Acid, 2% ultrapure water, 5mM ammonium formate
- Mobile phase B: 0.1% Formic acid in ultrapure water, 2% methanol, 5mM ammonium formate
- Flow rate: 0.3 mL/min
- Injection volume: 4 µL

Mobile phase gradient

Time [min]	Mobile phase A	Mobile phase B
0	20%	80%
2	20%	80%
15	100%	0%
17	100%	0%

Re-equilibration with initial mobile phase: 2.5 minutes.

3.2.2. Agilent 6550 LC-QTOF-MS

- 4GHz High Resolution Mode
- ESI source gas temperature: 160°C
- Gas flow: 14 L/min
- Nebuliser gas and collision gas: nitrogen
- Nebuliser gas pressure: 30 psi
- Sheath gas flow: 12 L/min
- Sheath gas temperature: 350 °C
- Ionisation mode: positive
- Capillary voltage: 4000 V
- OctapoleRFPeak 750V
- Fragmentor 360 V

3.3 Data processing

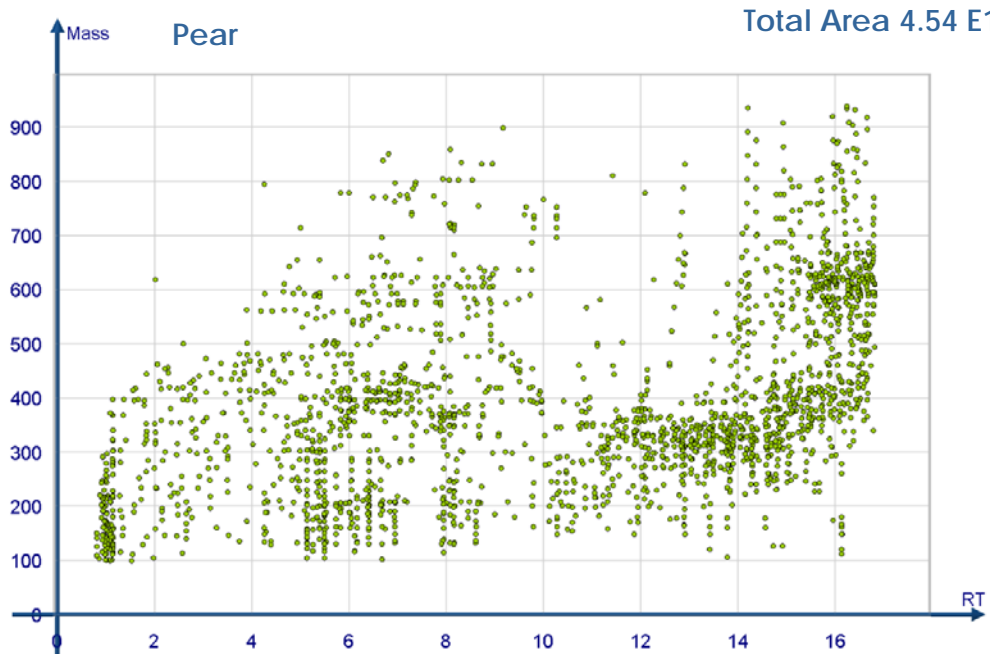
MS data were processed and evaluated using the statistical software Agilent Mass Profiler Professional (MPP)13.0. The graphical representation of the molecular component map was carried out using the visual data mining software Miner 3D Enterprise 7

4. Number and distribution of co-extracted matrix components

4.1 High water content

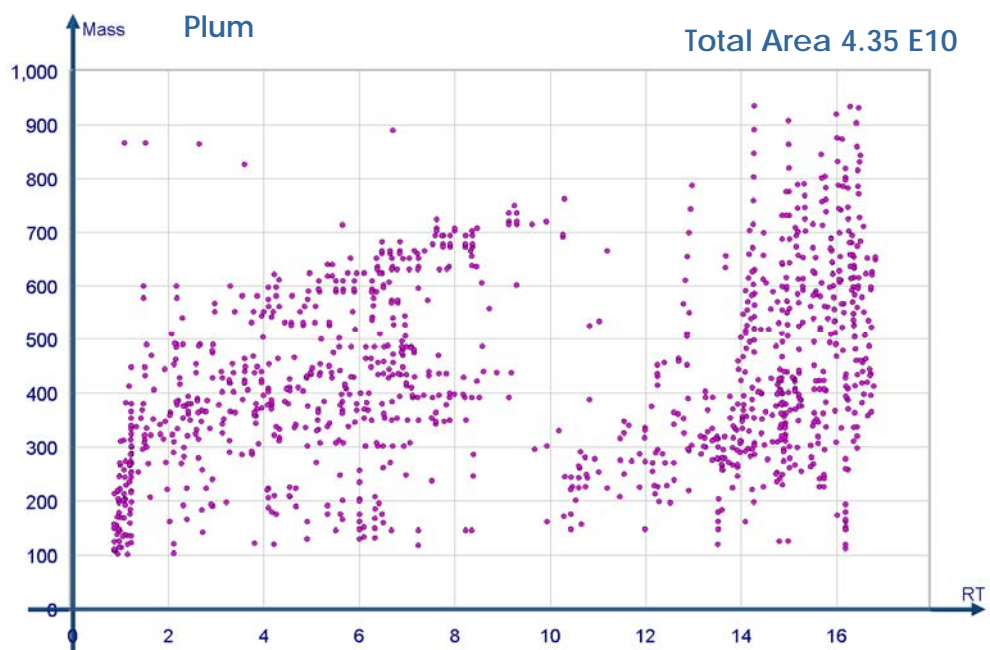
- Pome fruit

1354 Matrix compounds

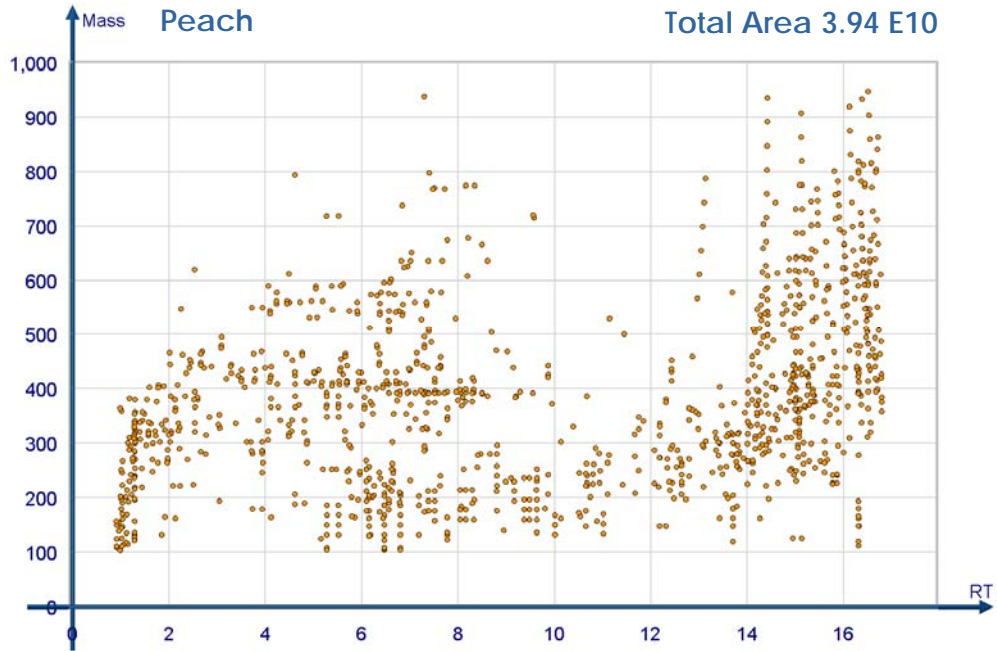


- Stone fruit

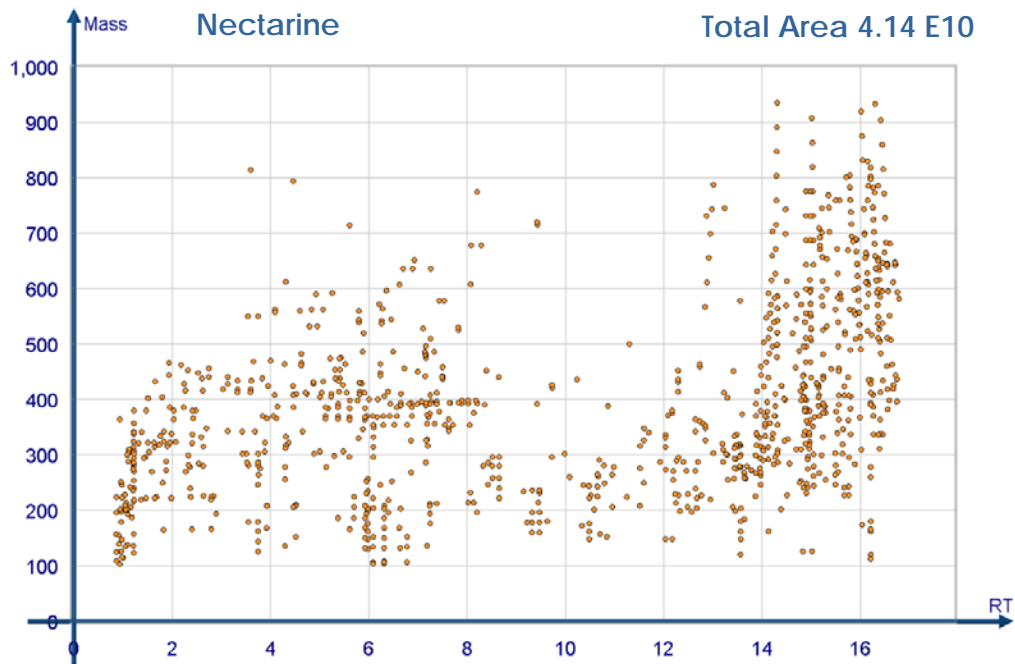
1156 Matrix compounds



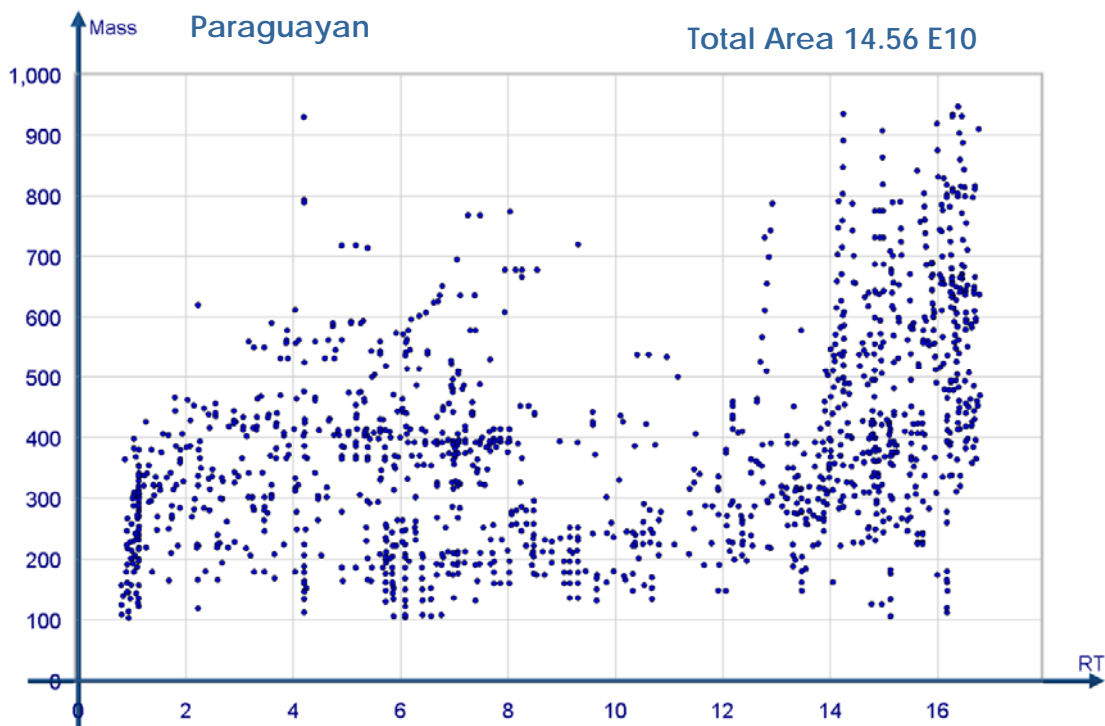
1187 Matrix compounds



1002 Matrix compounds

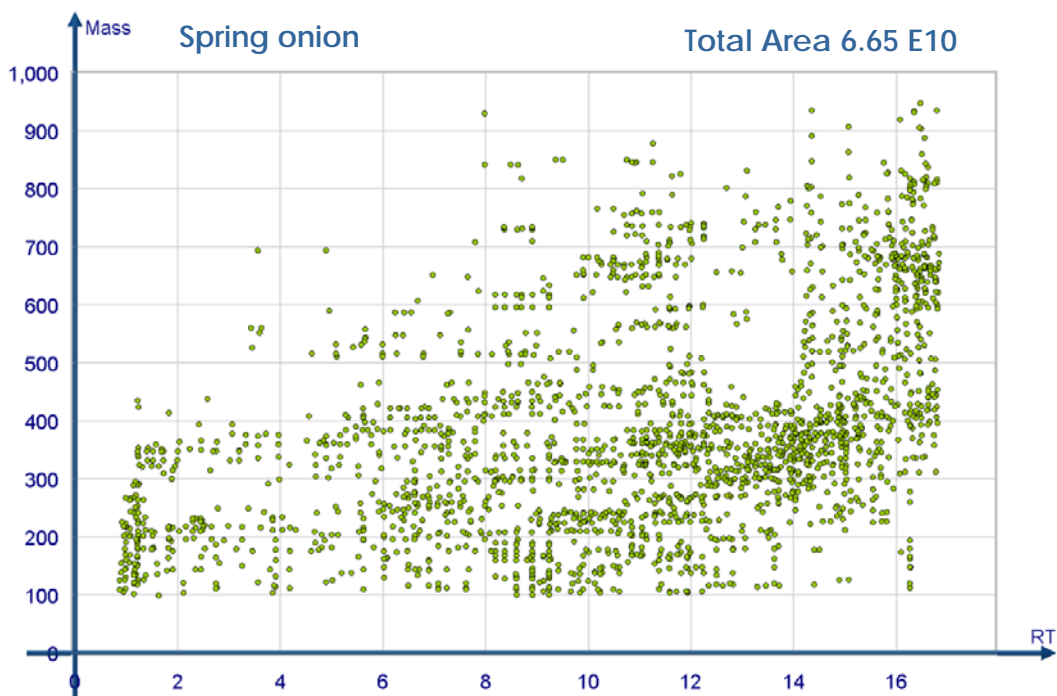


1360 Matrix compounds



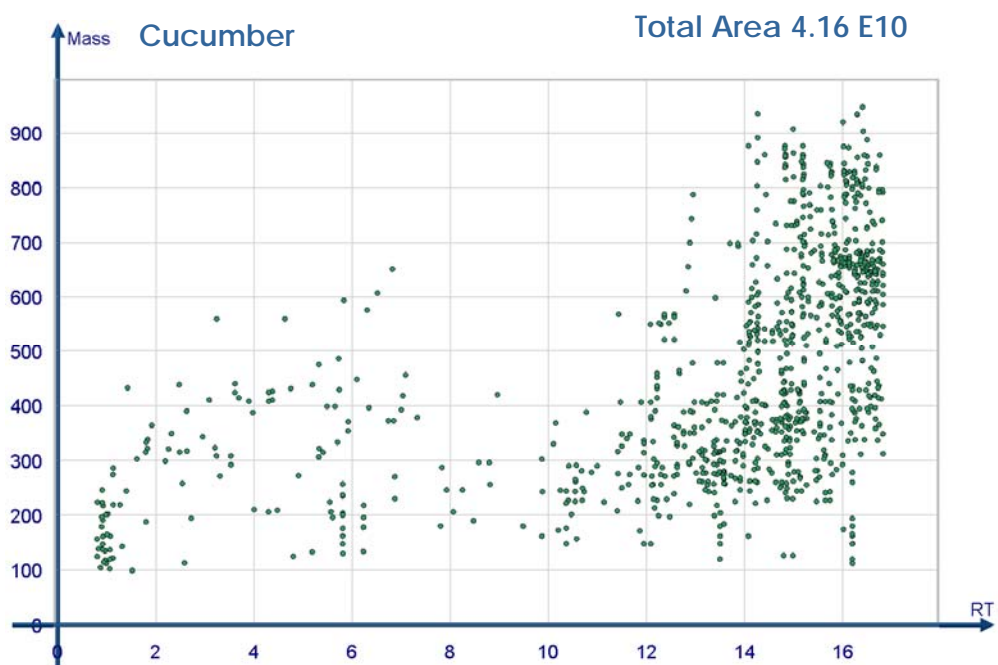
▪ Alliums

2256 Matrix compounds

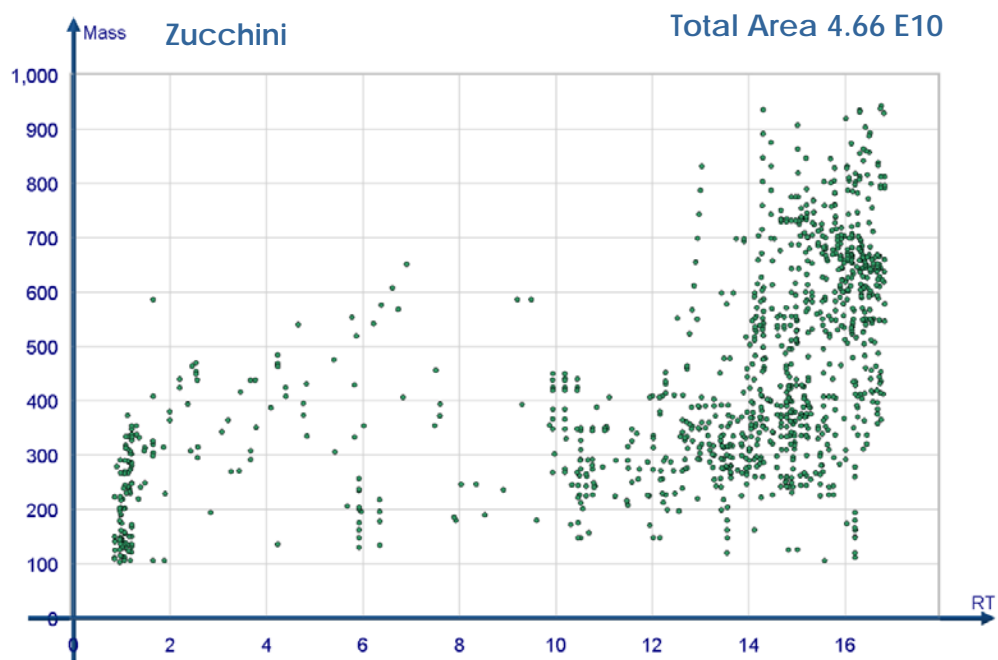


- Fruiting vegetables/cucurbits

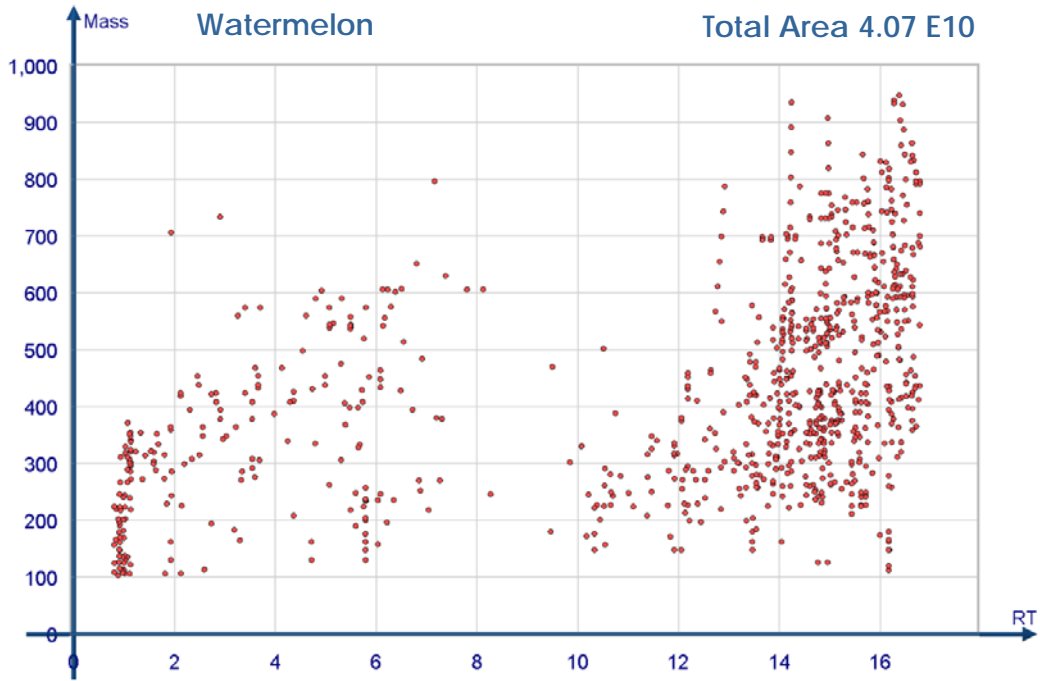
993 Matrix compounds



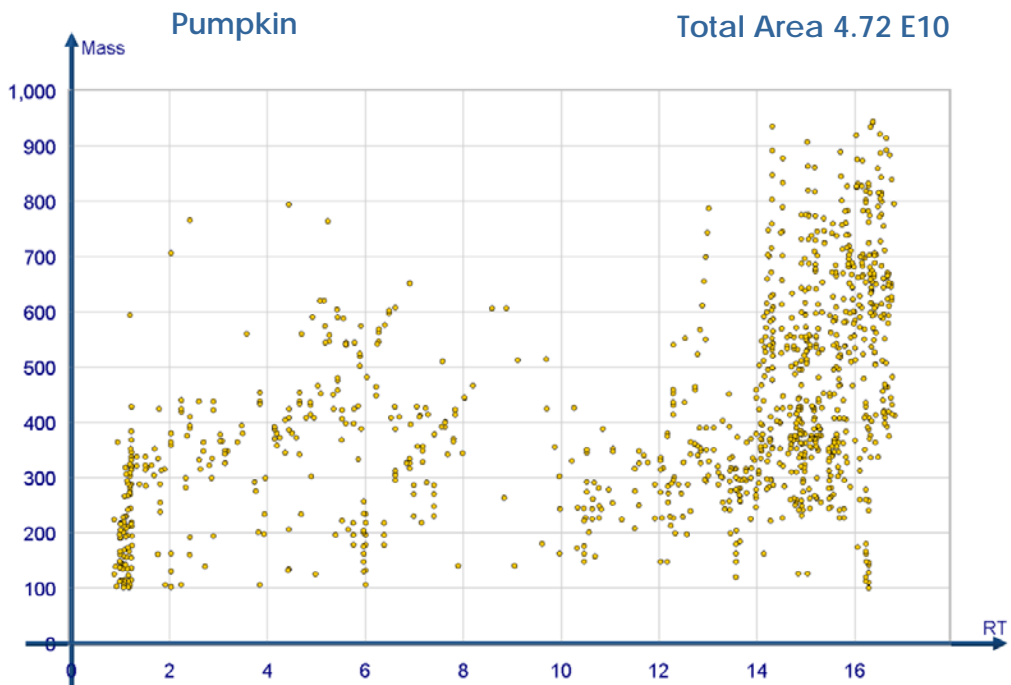
1083 Matrix compounds



890 Matrix compounds

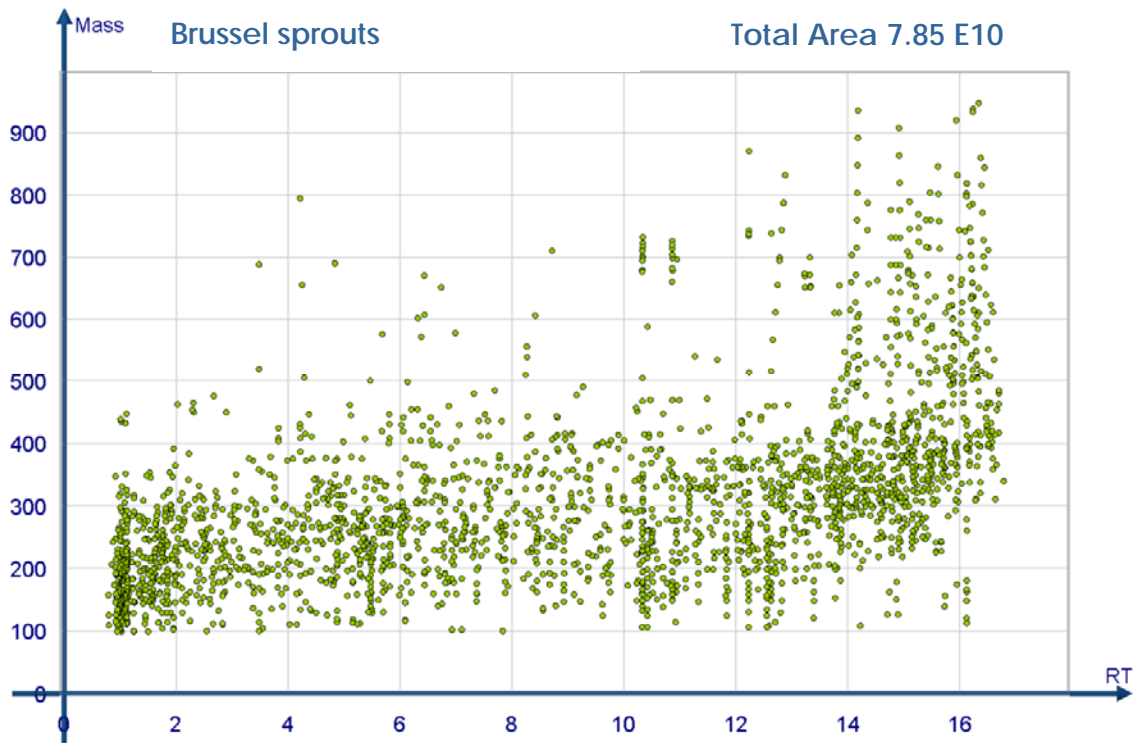


1059 Matrix compounds

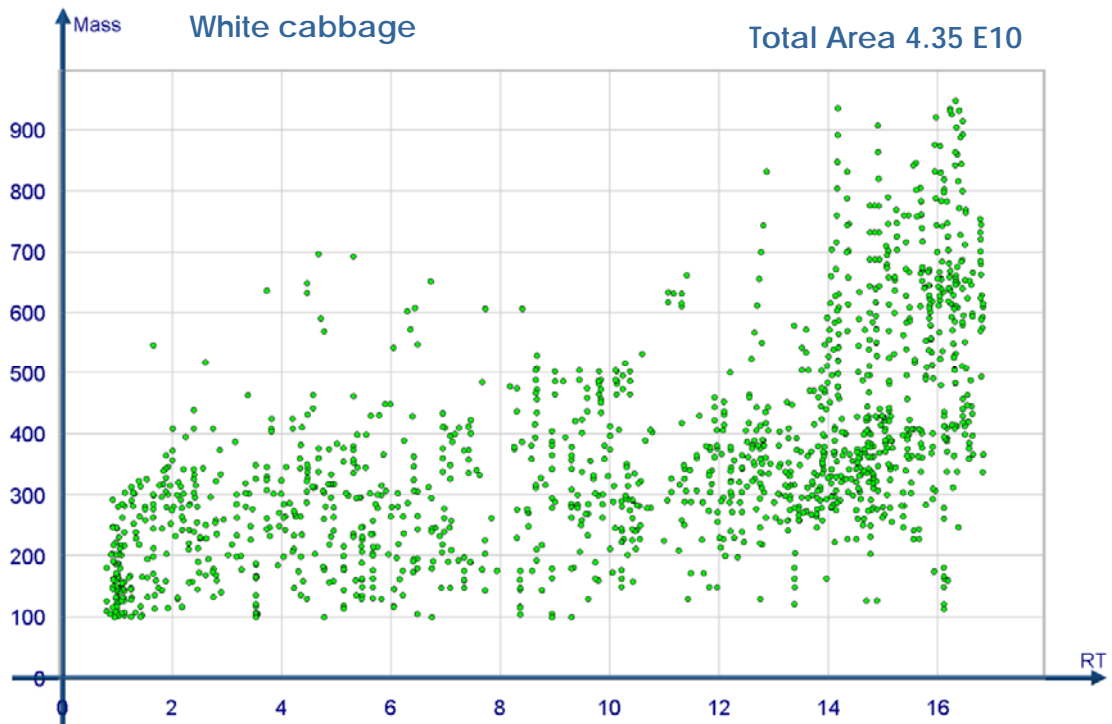


- Brassica vegetables

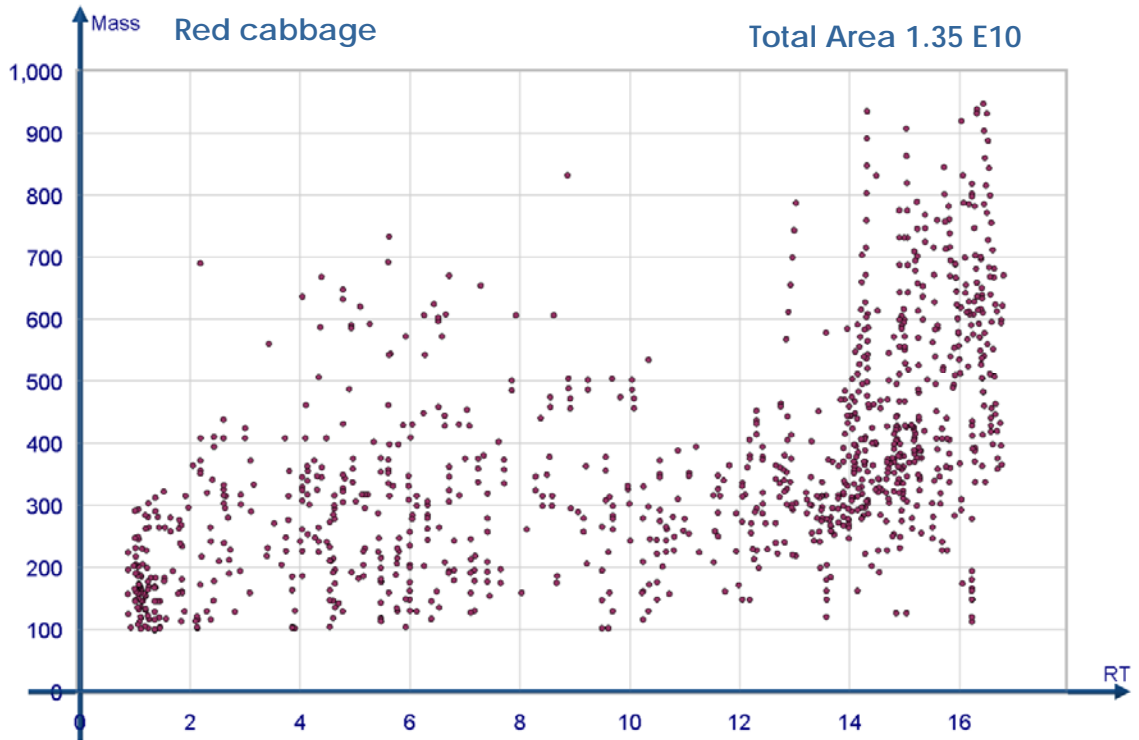
2470 Matrix compounds



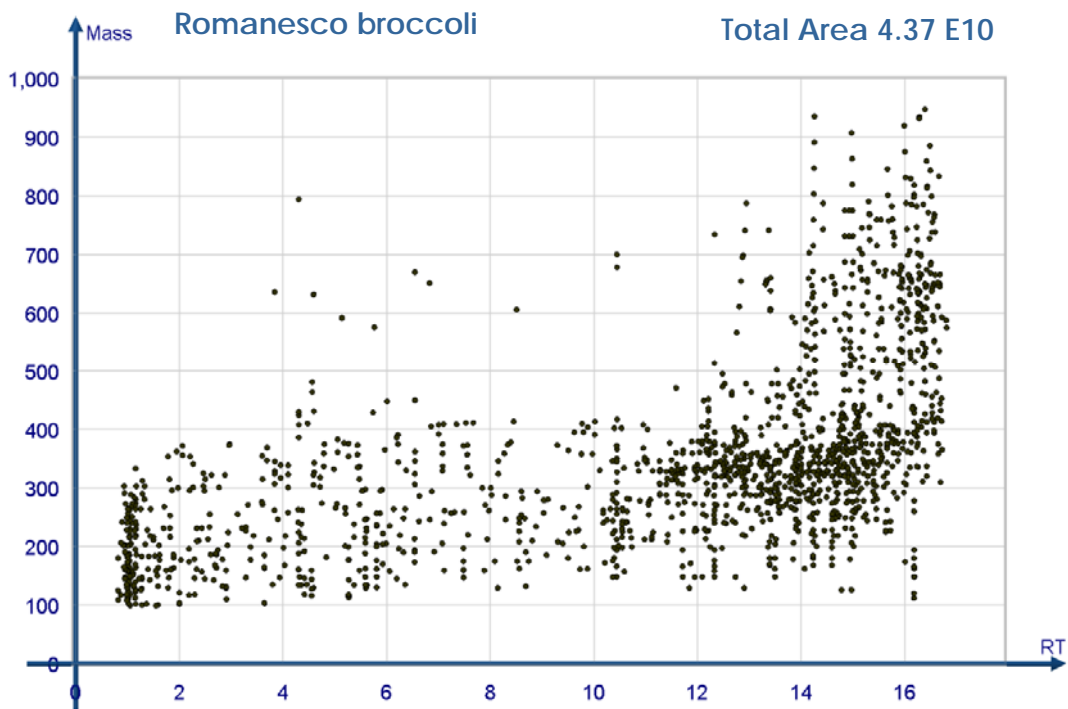
1429 Matrix compounds



1074 Matrix compounds

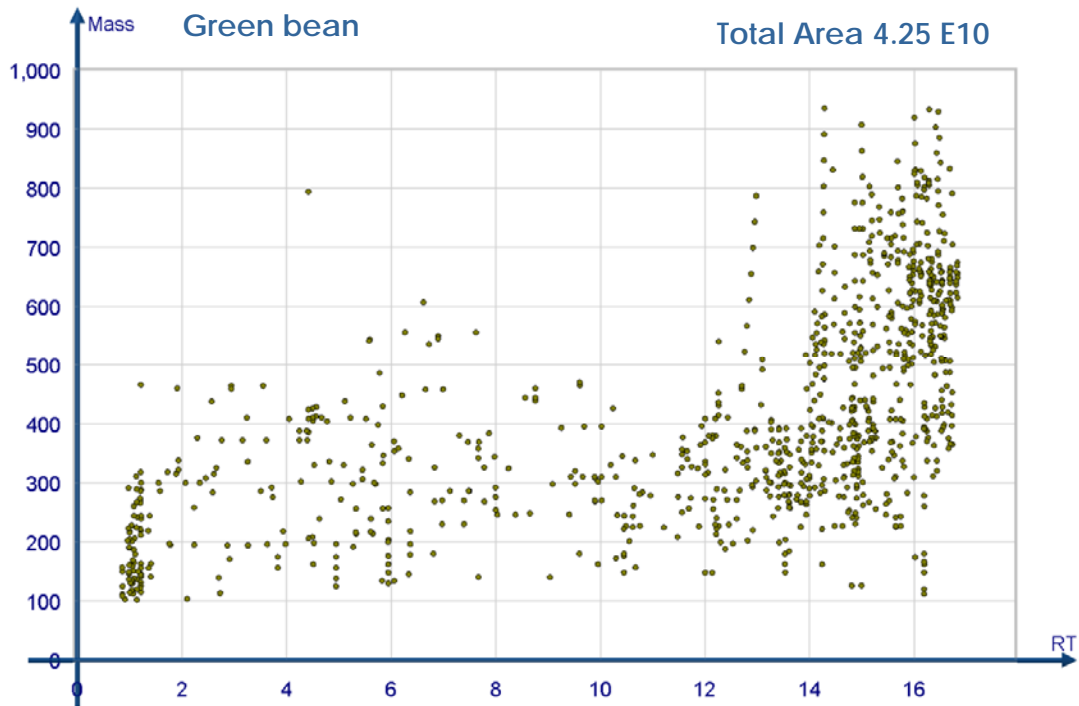


1622 Matrix compounds



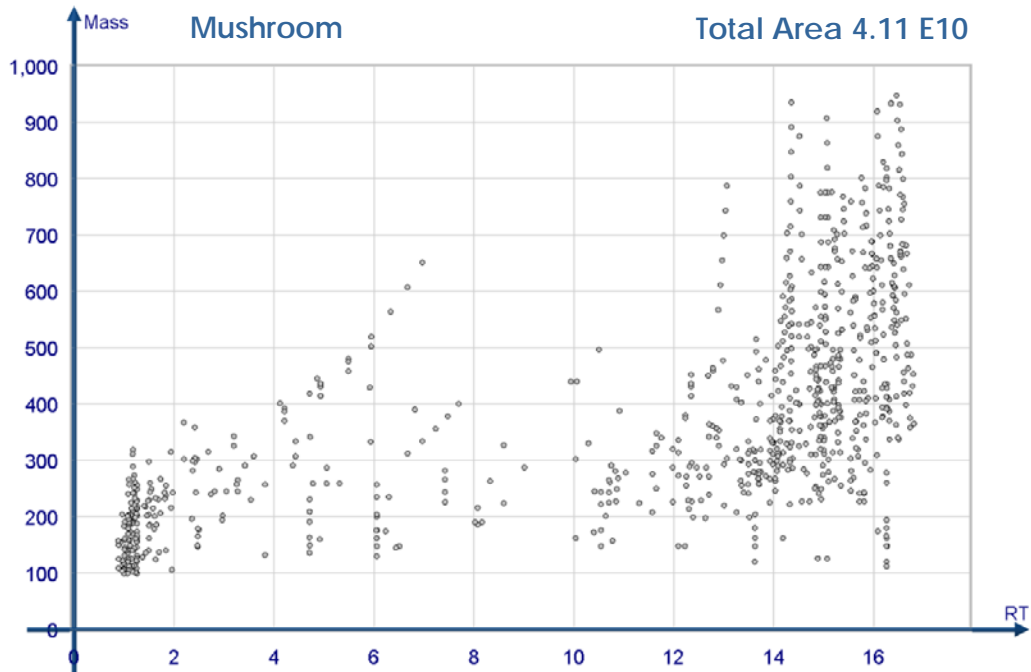
- Fresh legume vegetables

955 Matrix compounds



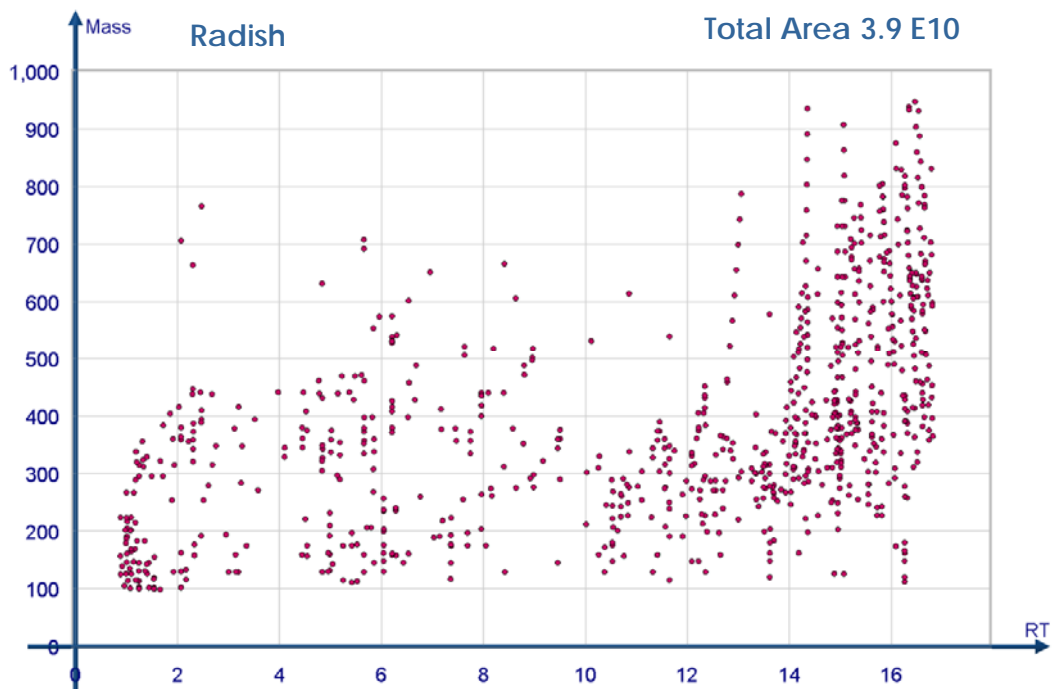
- Fresh fungi

1187 Matrix compounds

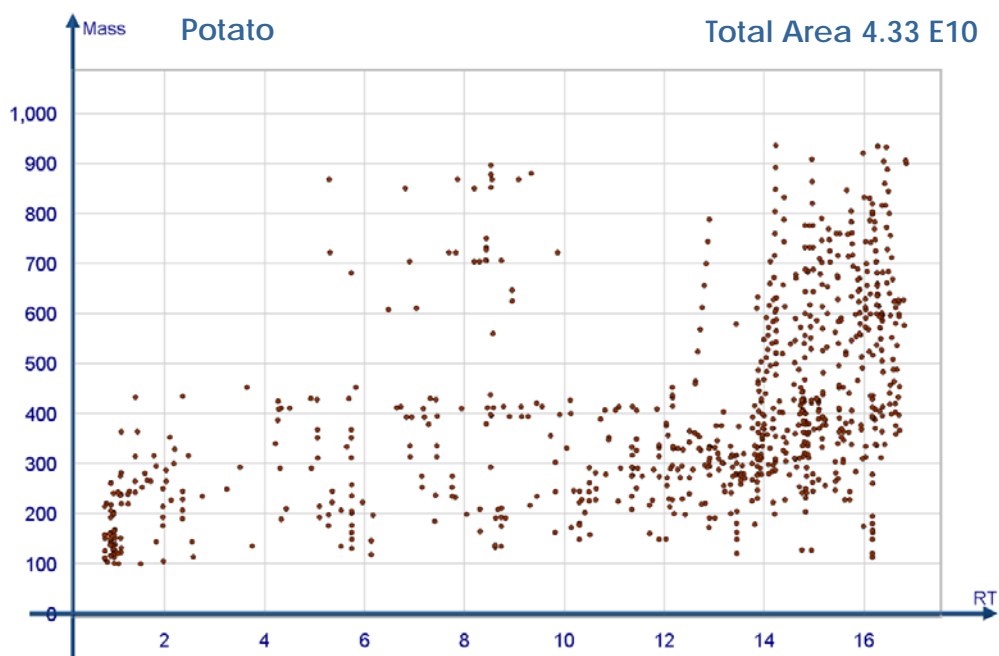


- Root and tuber vegetables or feed

860 Matrix compounds

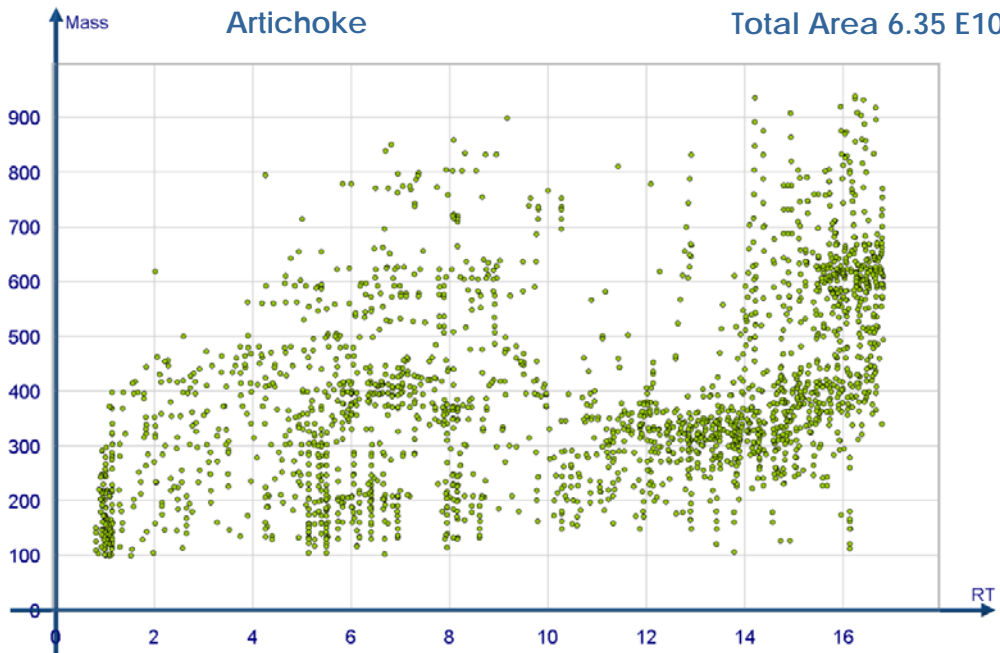


837 Matrix compounds

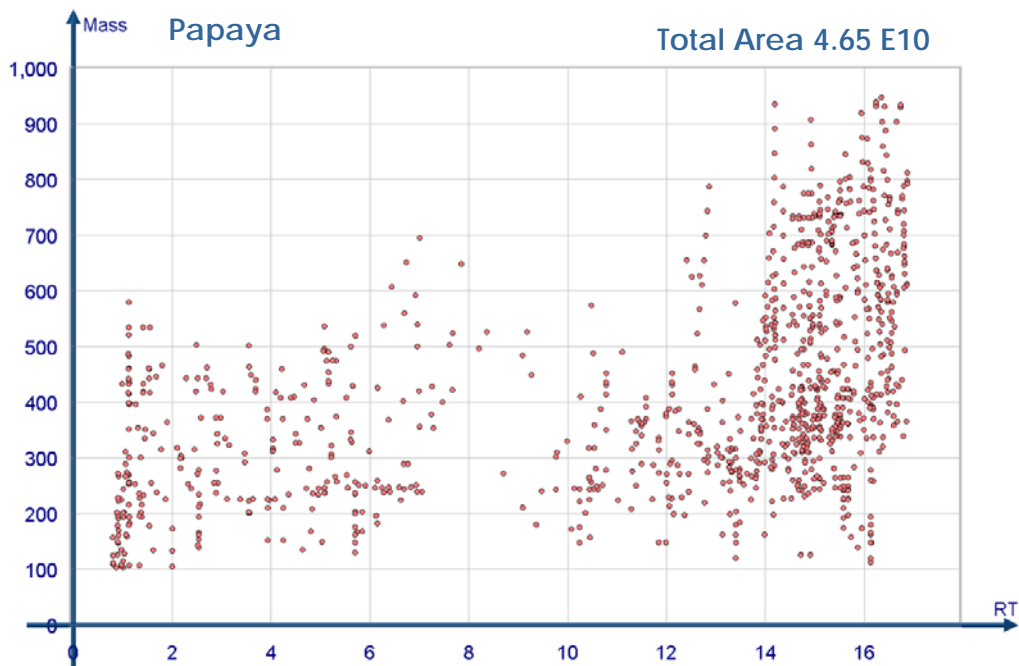


Other

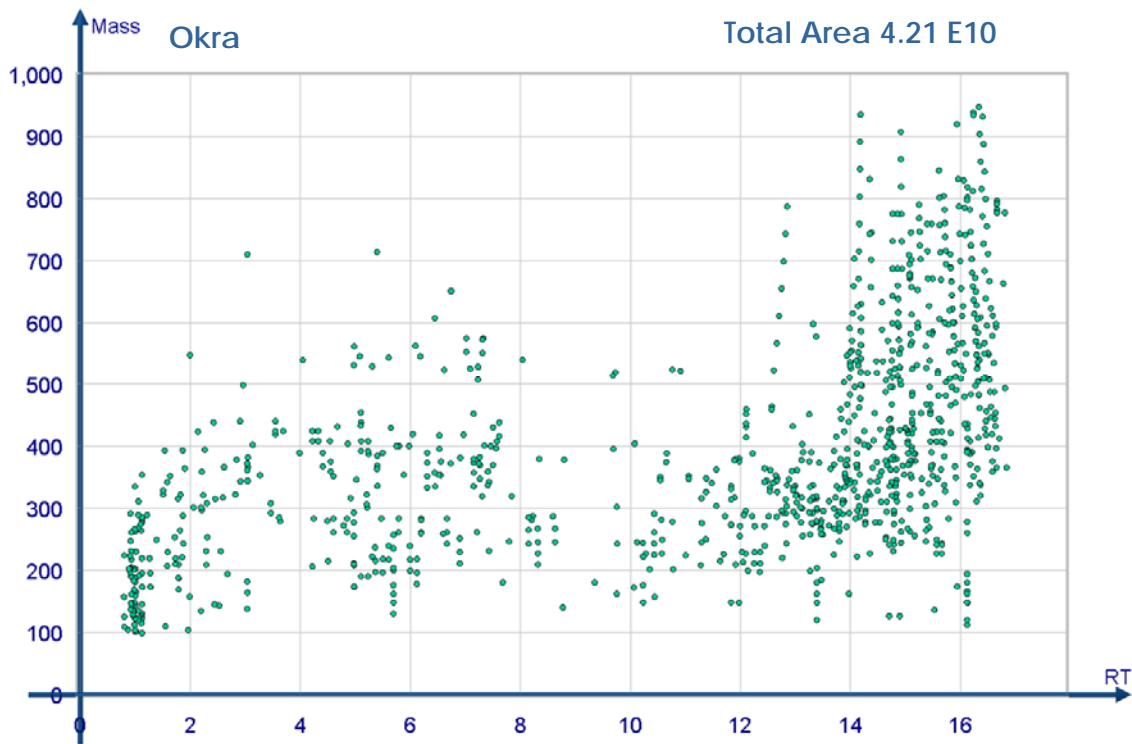
2206 Matrix compounds



1069 Matrix compounds



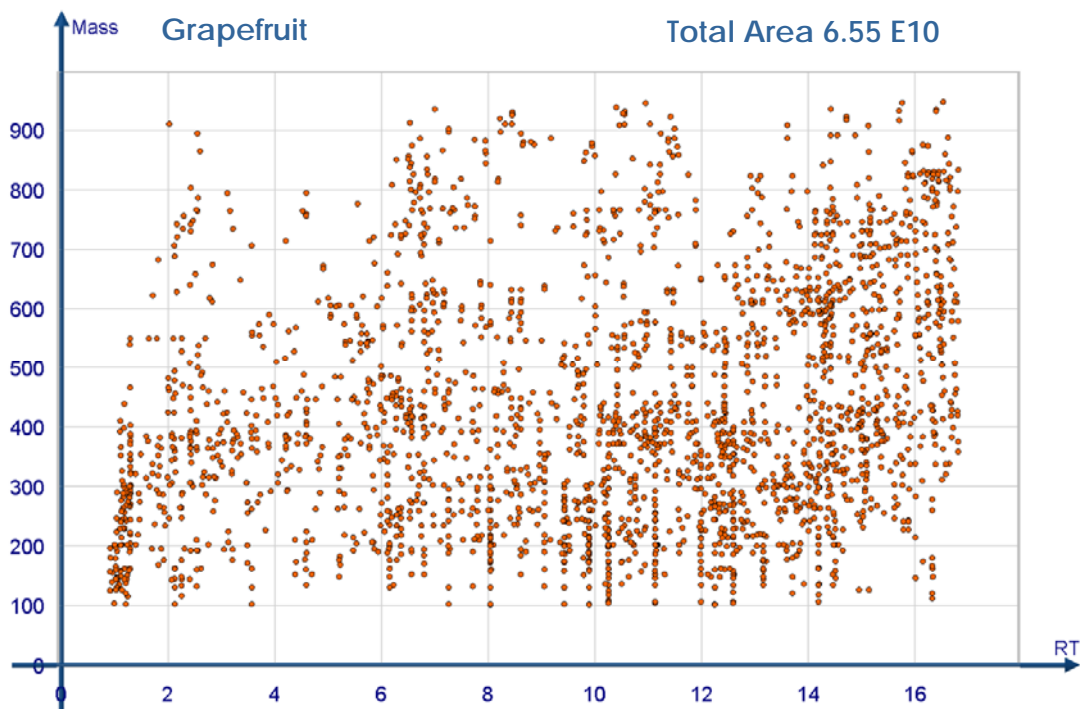
1028 Matrix compounds



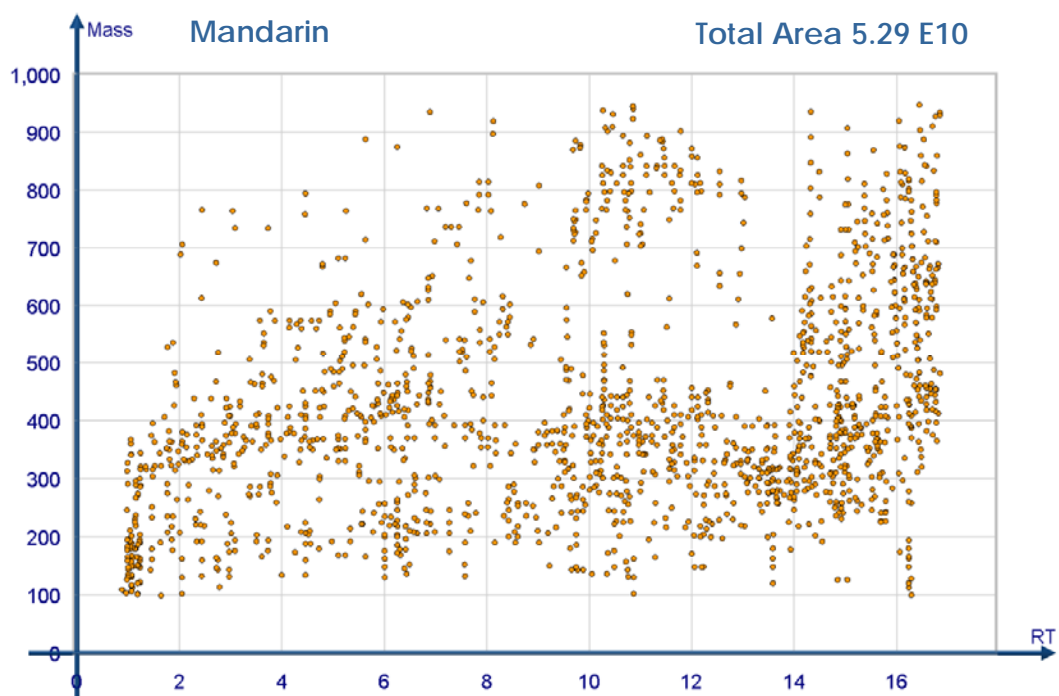
4.2 High acid content and high water content

- Citrus fruit

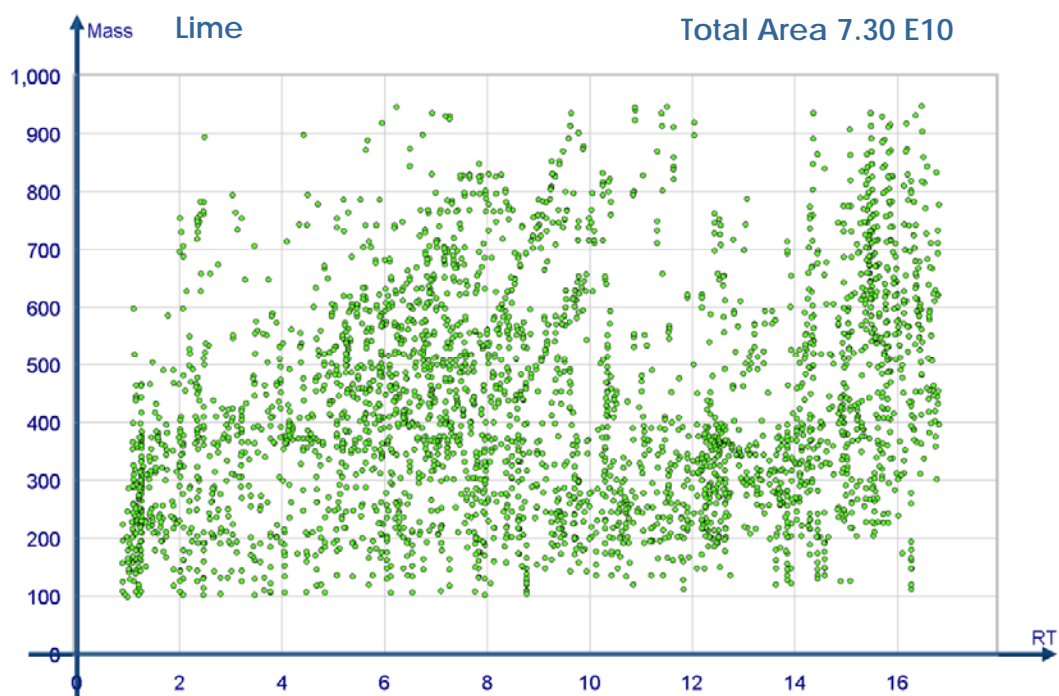
2565 Matrix compounds



1692 Matrix compounds

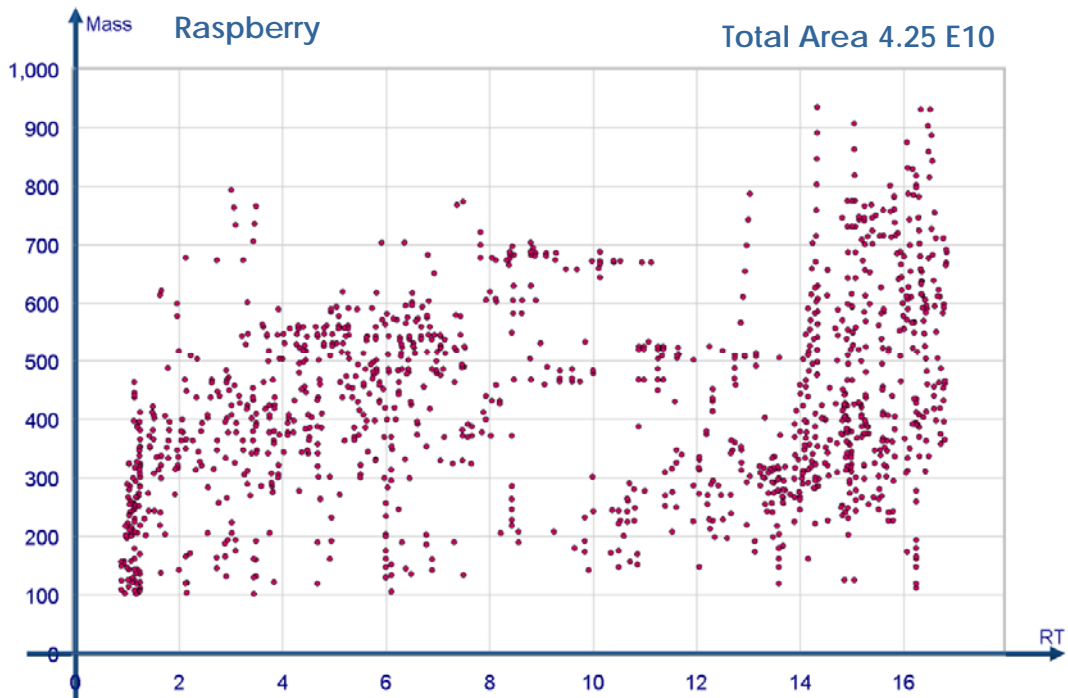


3345 Matrix compounds



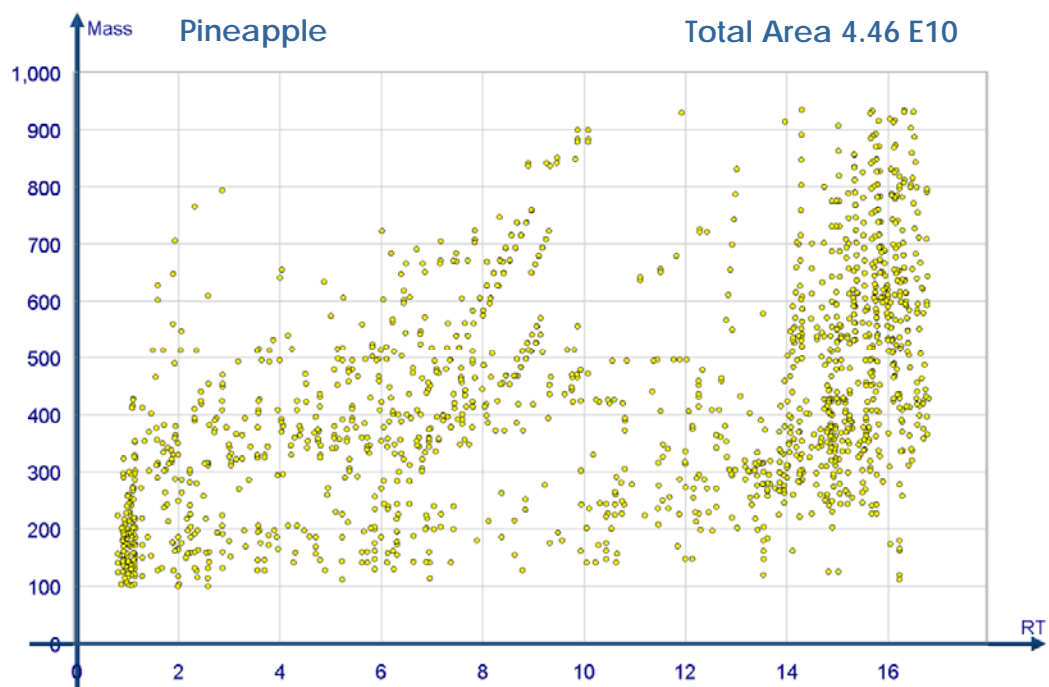
- Small fruit and berries

1247 Matrix compounds

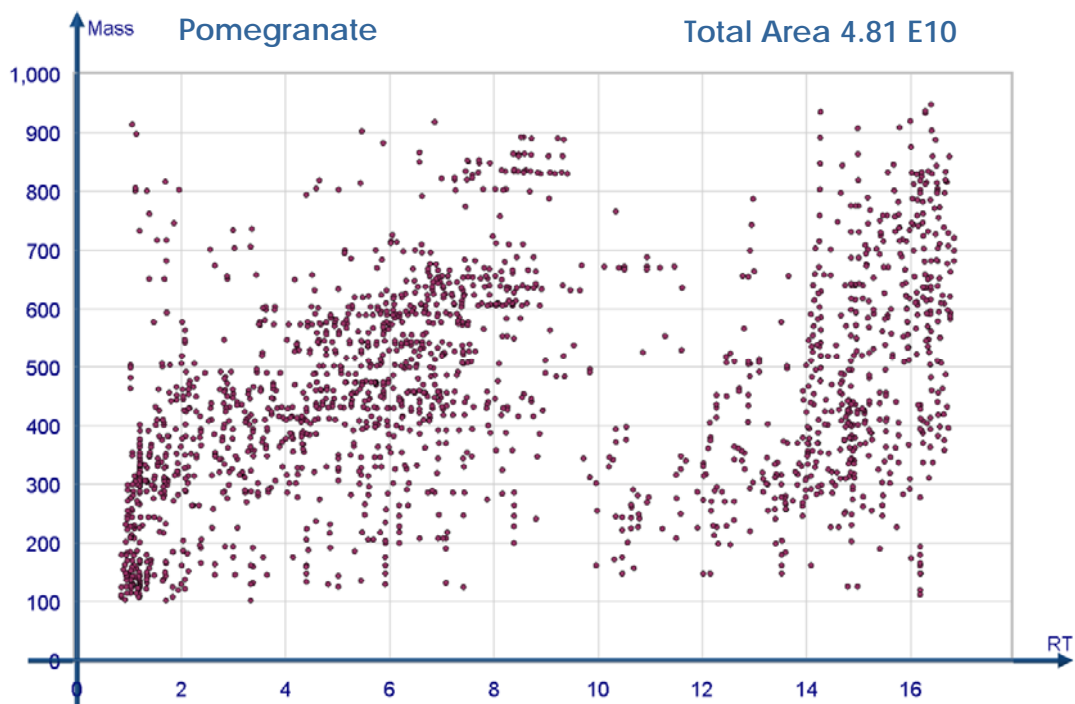


- Other

837 Matrix compounds

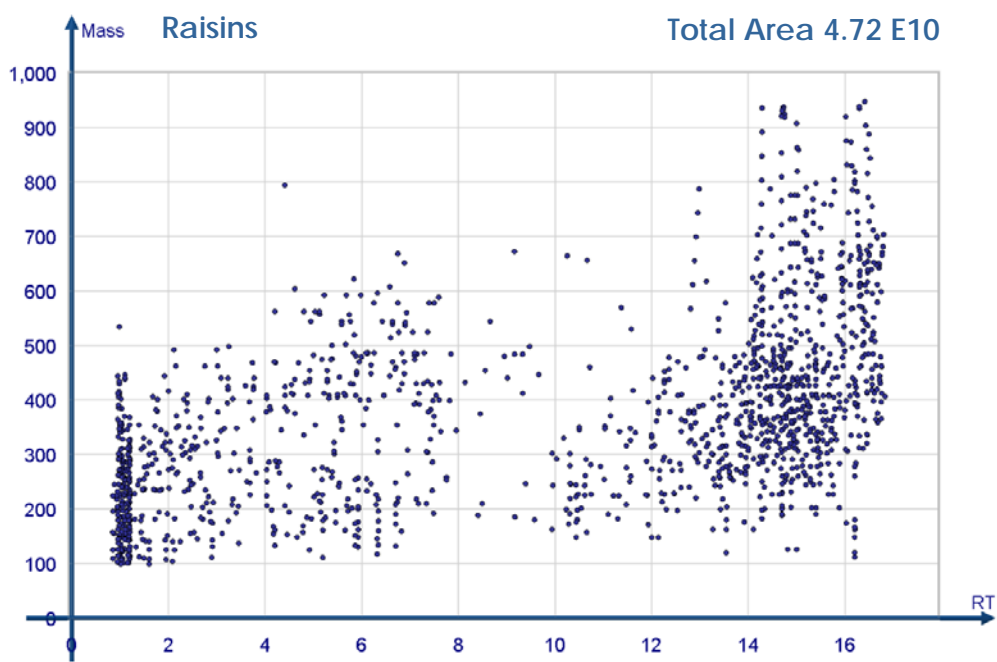


1829 Matrix compounds



4.3 High sugar and low water content

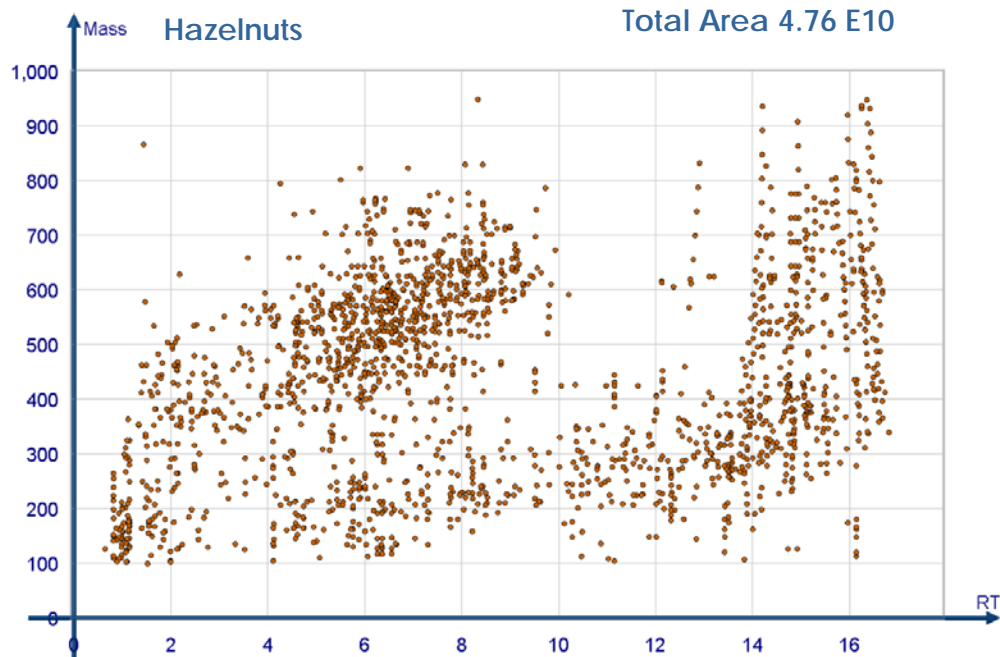
1468 Matrix compounds



4.4 High oil content and very low water content

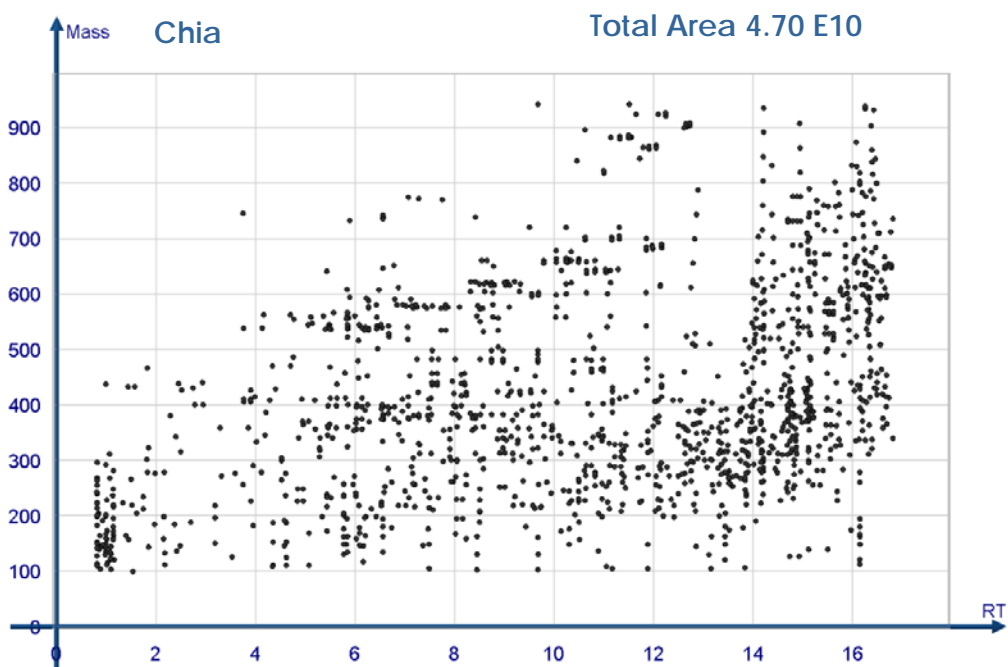
- Tree nuts

1908 Matrix compounds

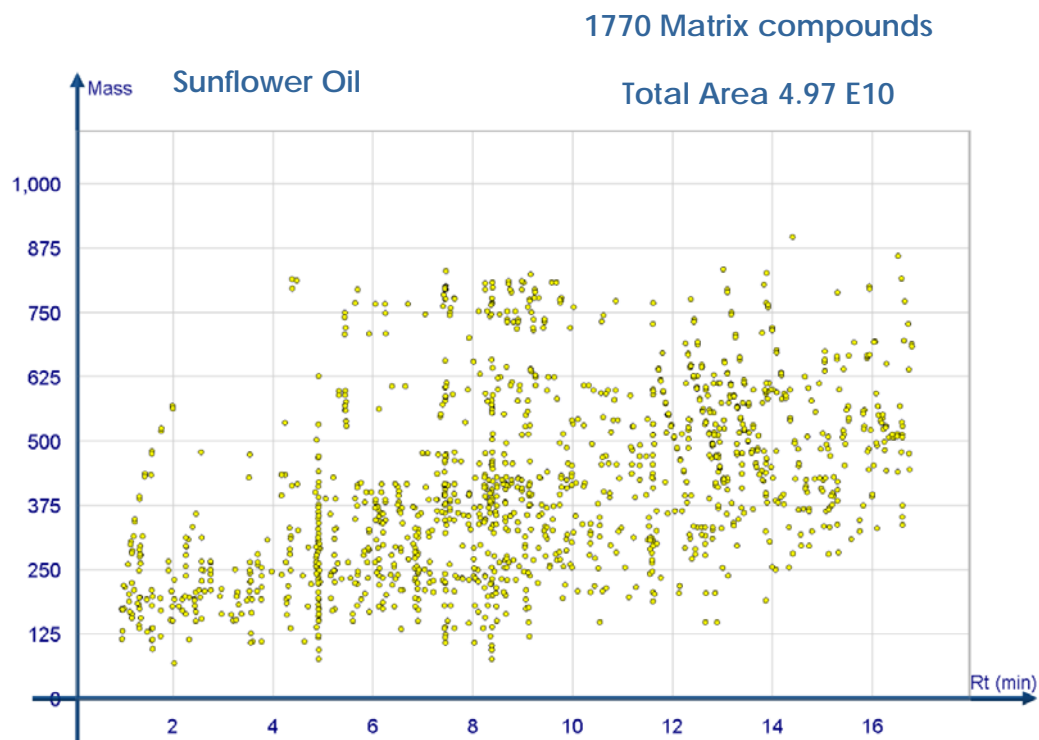
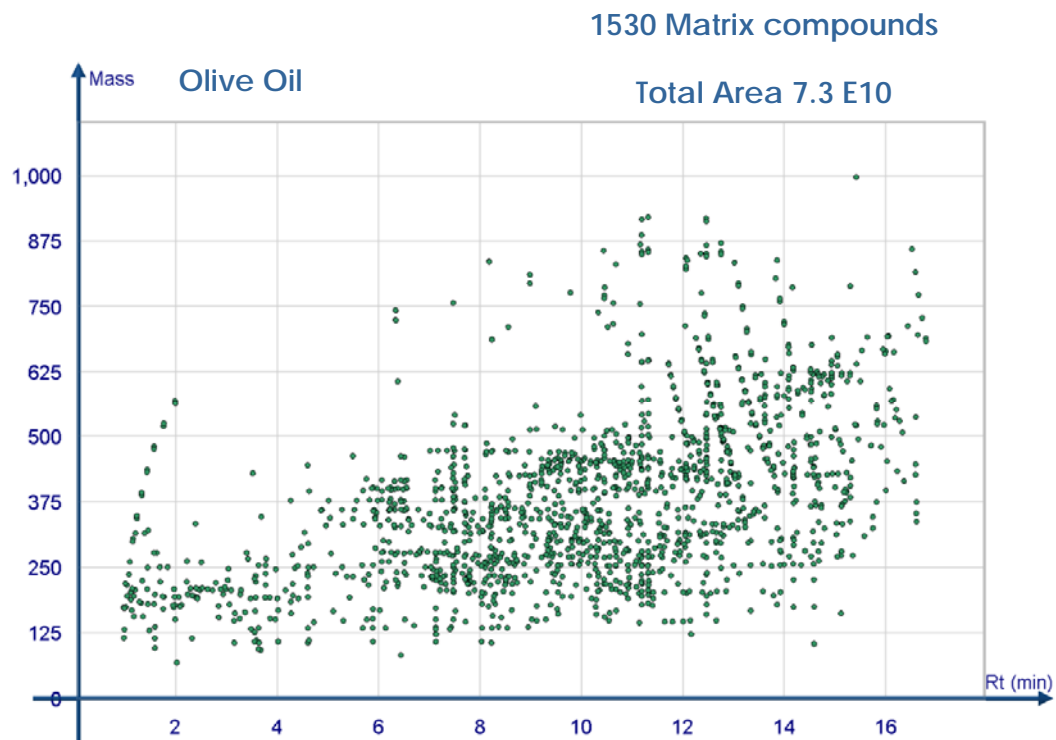


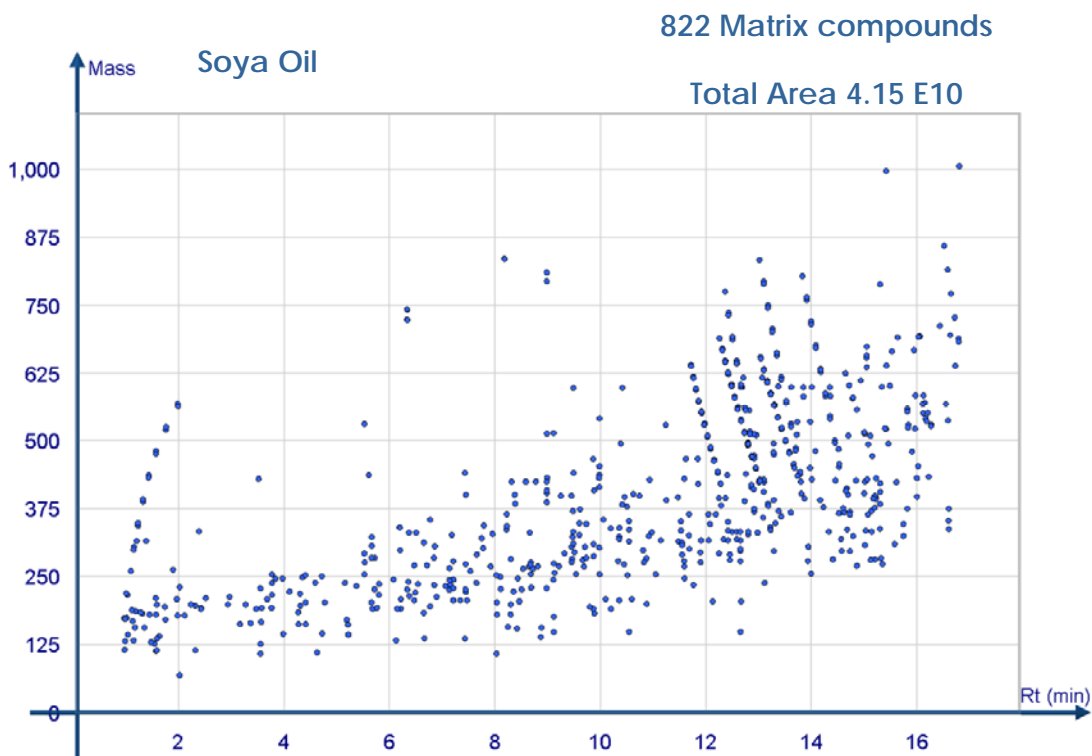
- Oil seeds

1443 Matrix compounds

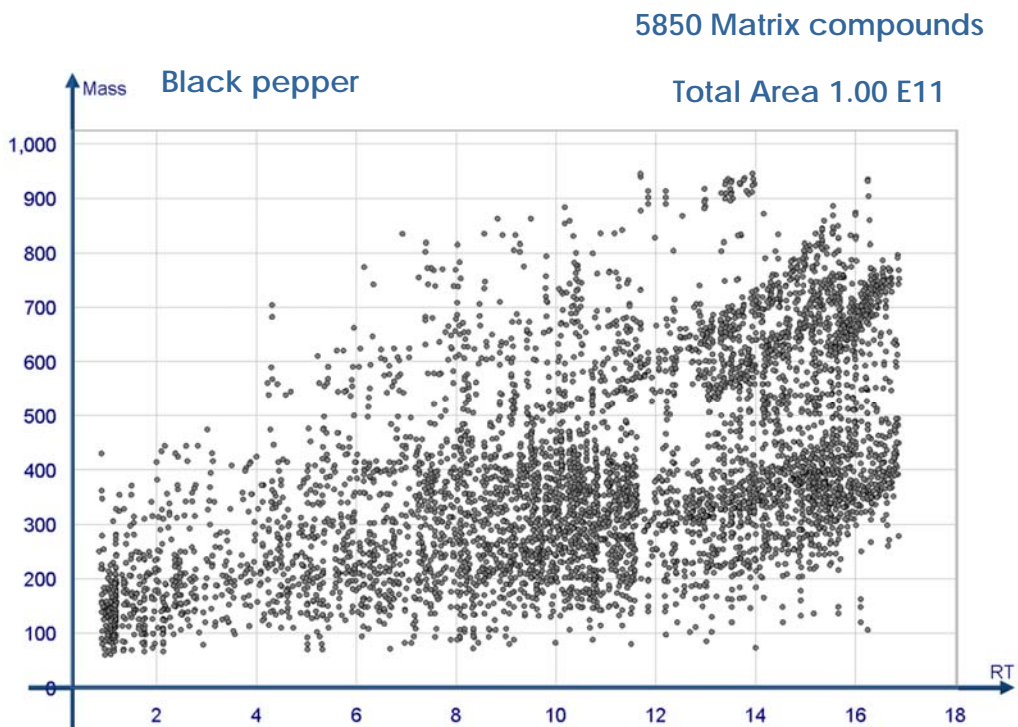


- Oils from tree nuts, oil seeds and oily fruits

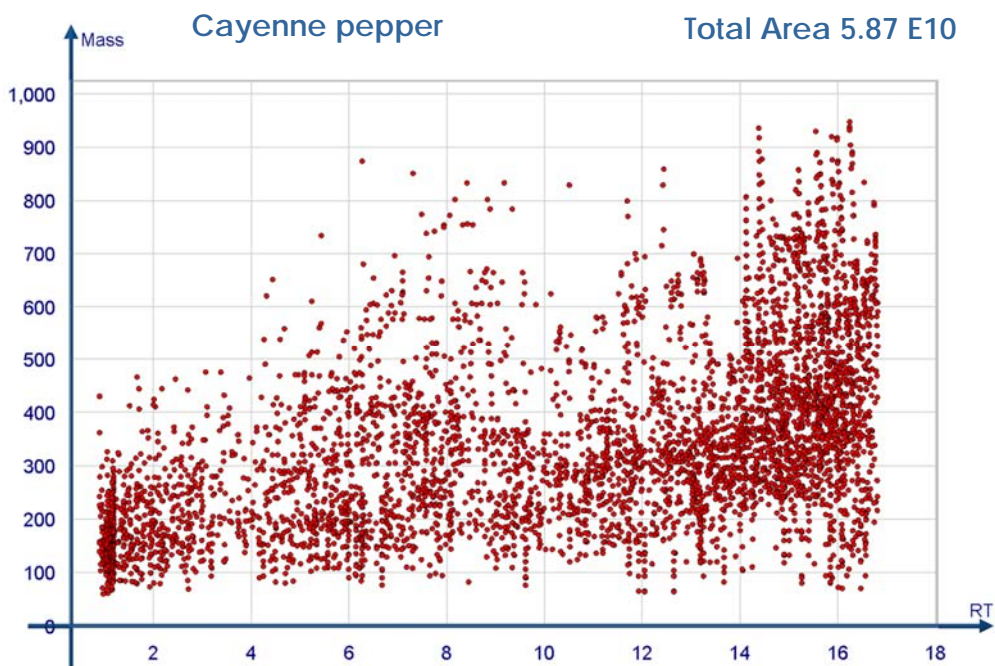




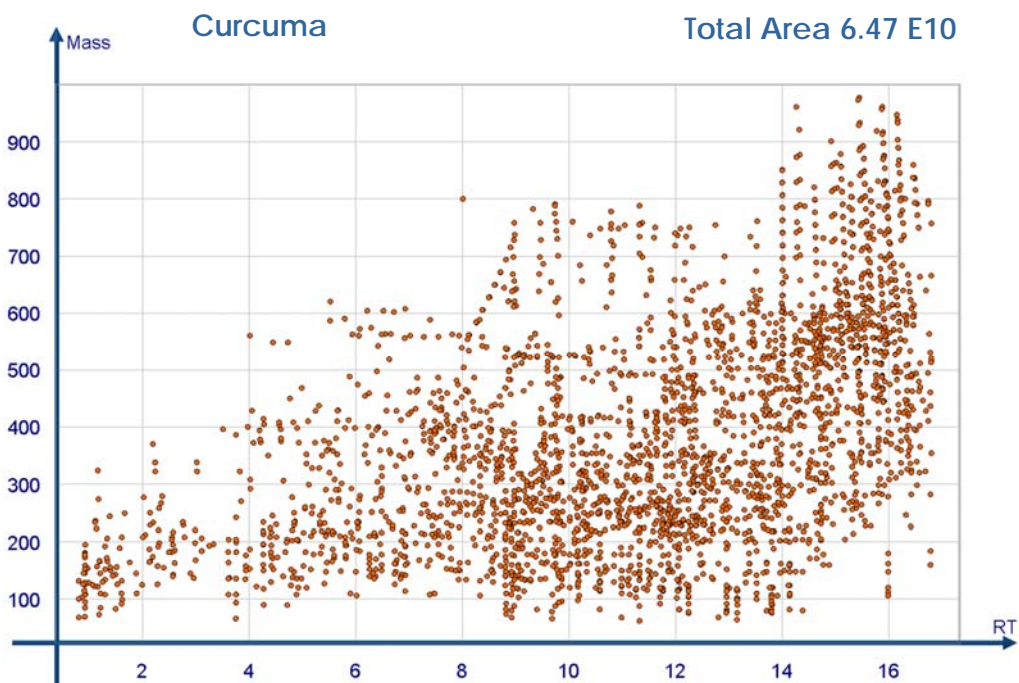
4.5 "Difficult or unique commodities"



4829 Matrix compounds

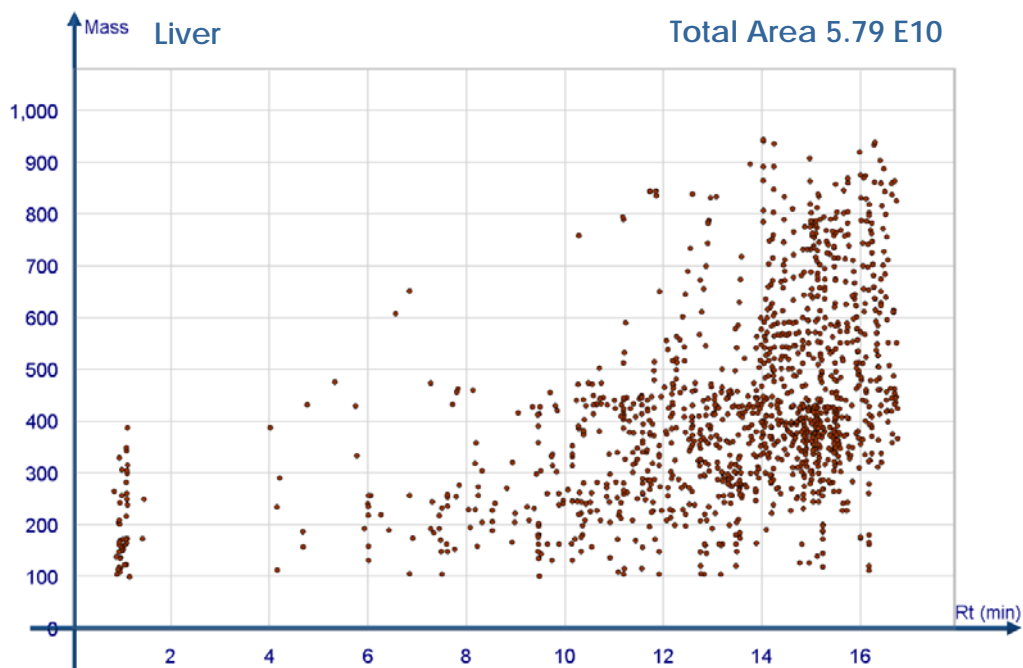


3972 Matrix compounds



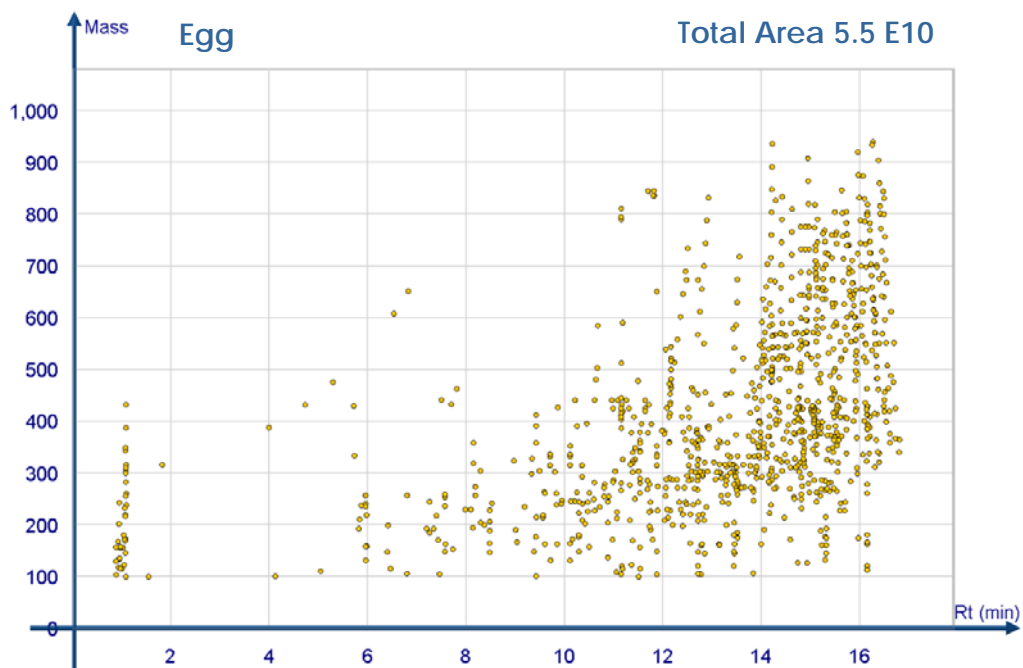
4.6 Meat and seafood

1302 Matrix compounds

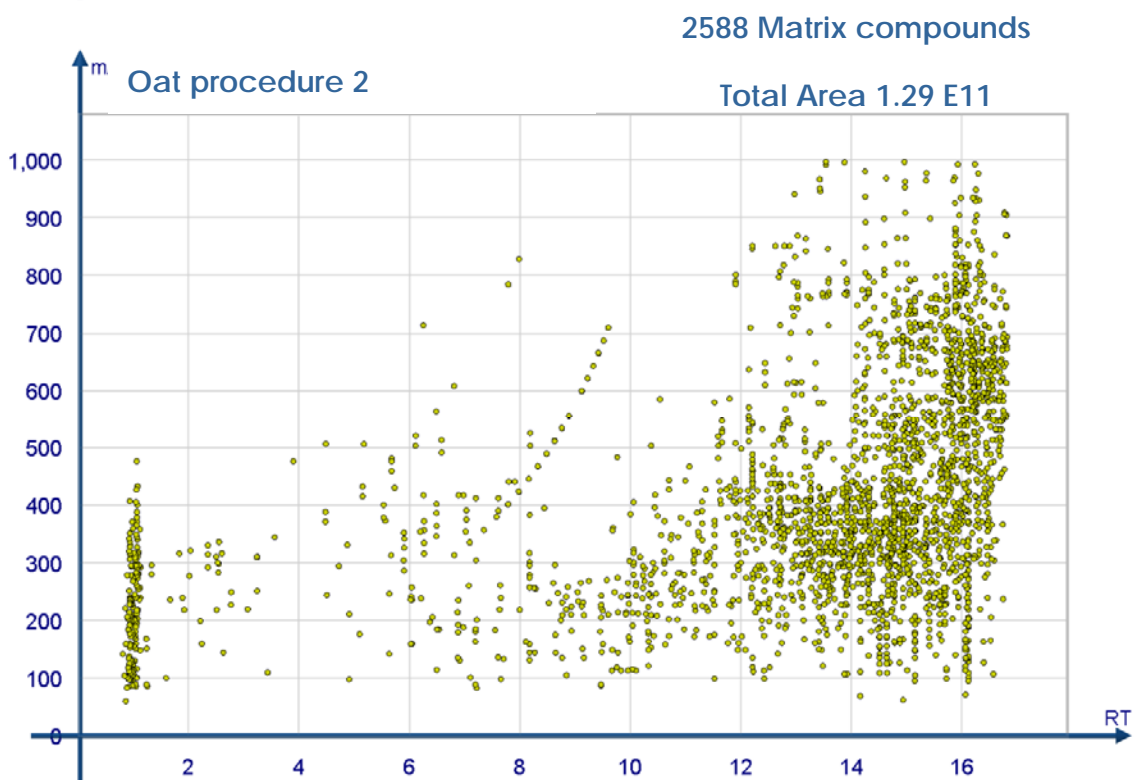
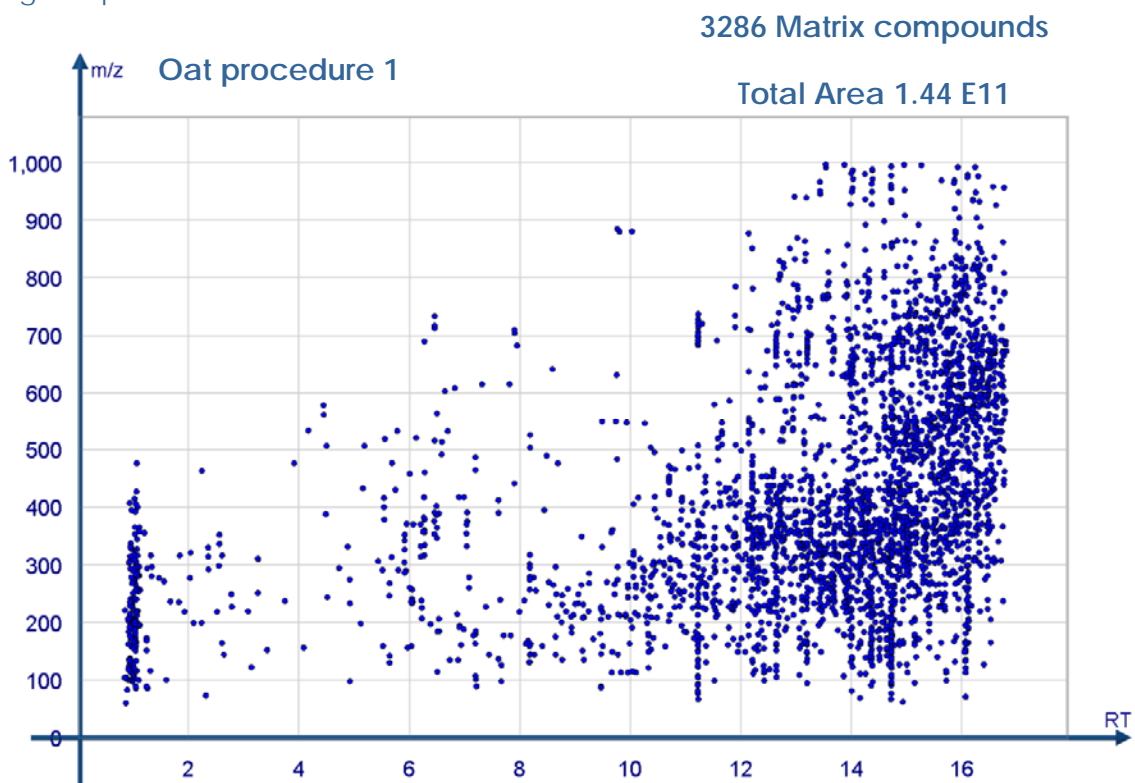


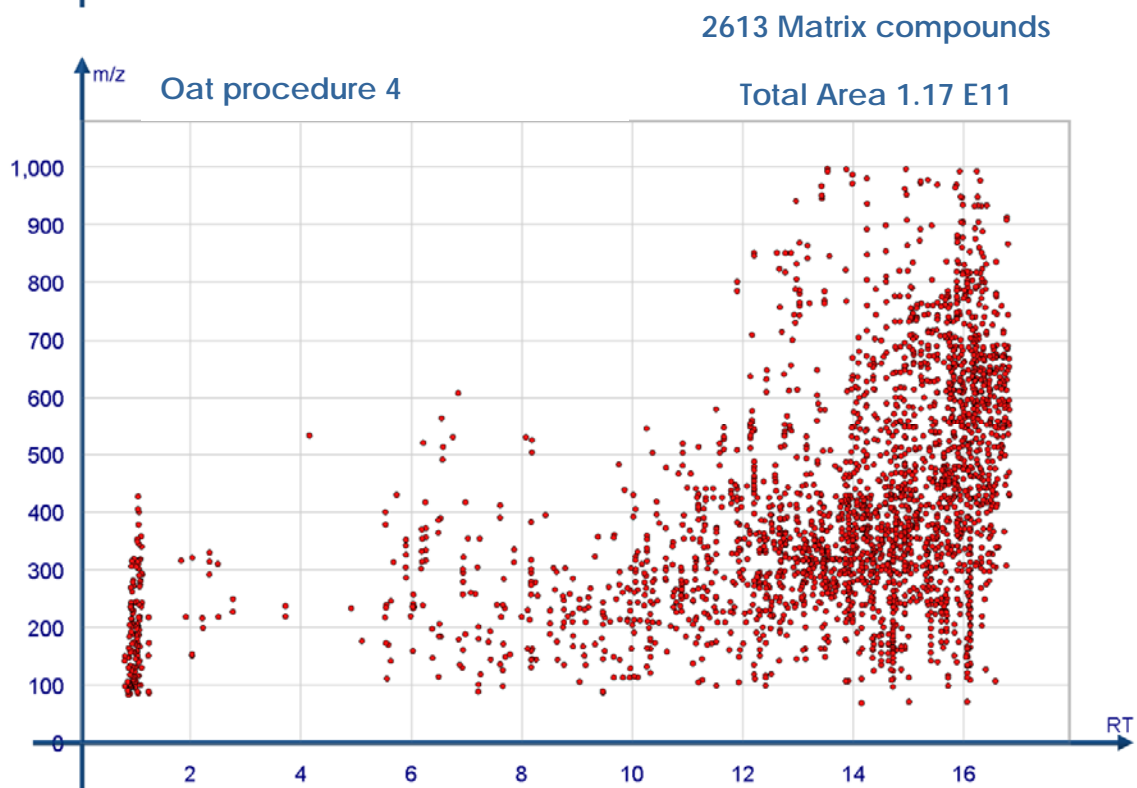
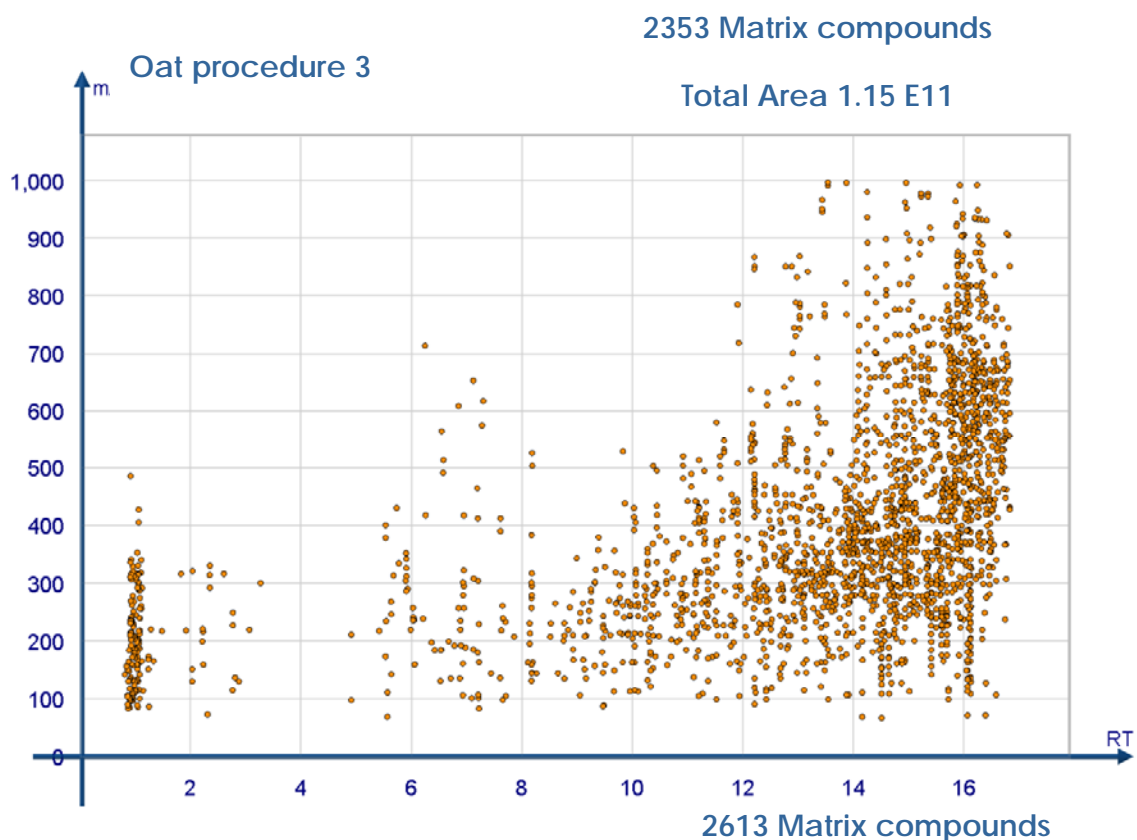
4.7 Eggs

1031 Matrix compounds

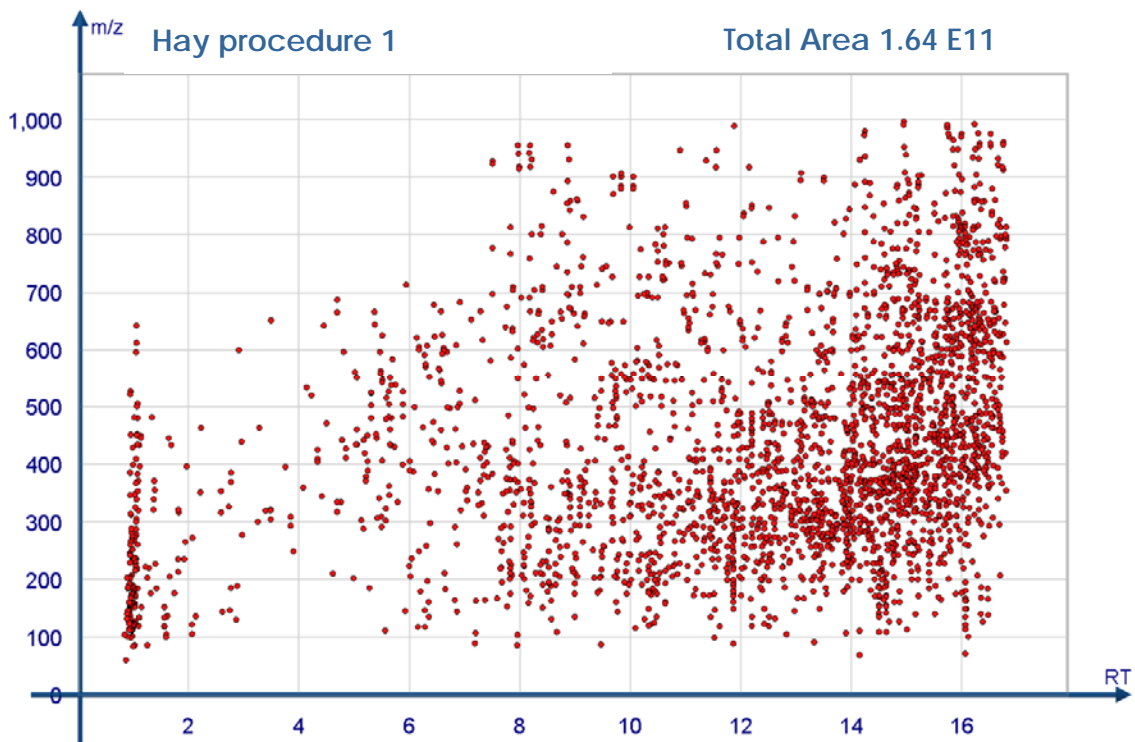


4.8 High starch and/or protein content and low water and fat content
1g sample/ml

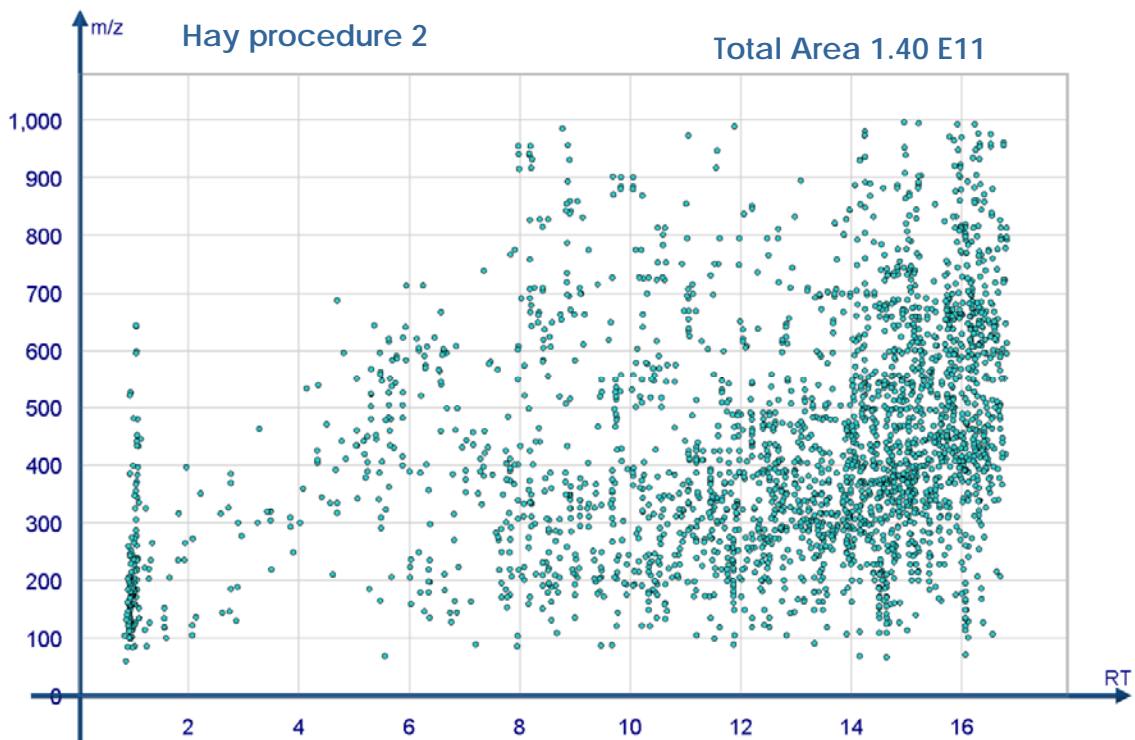




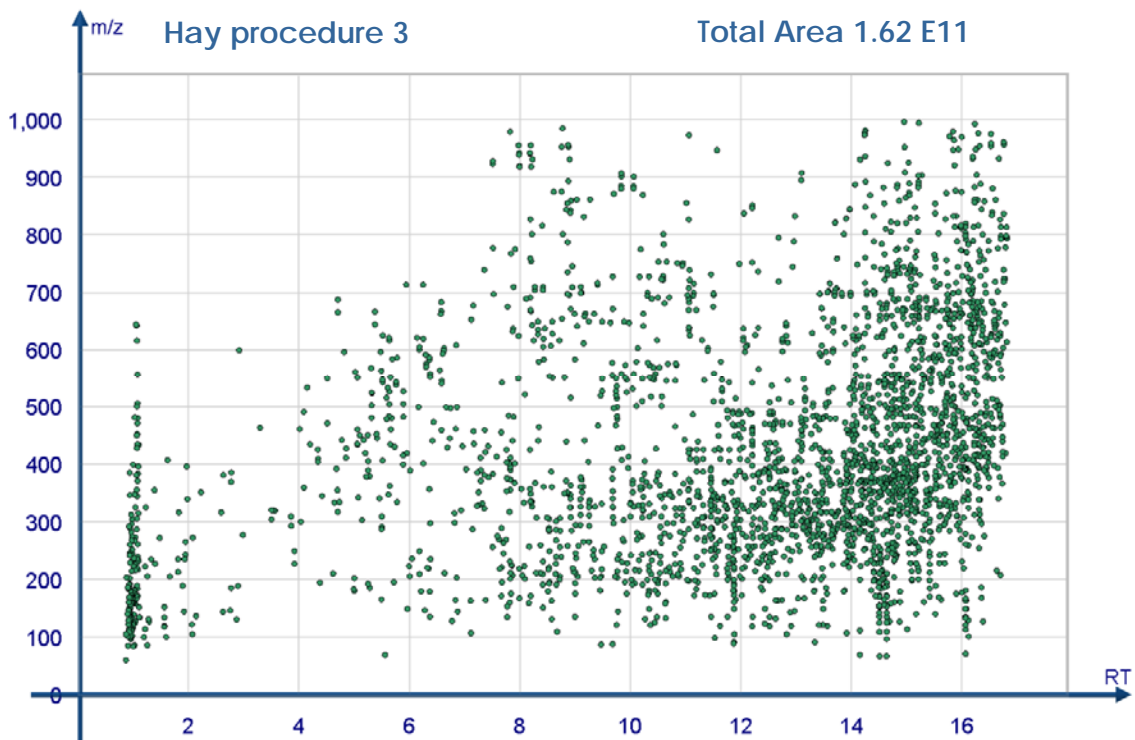
2904 Matrix compounds



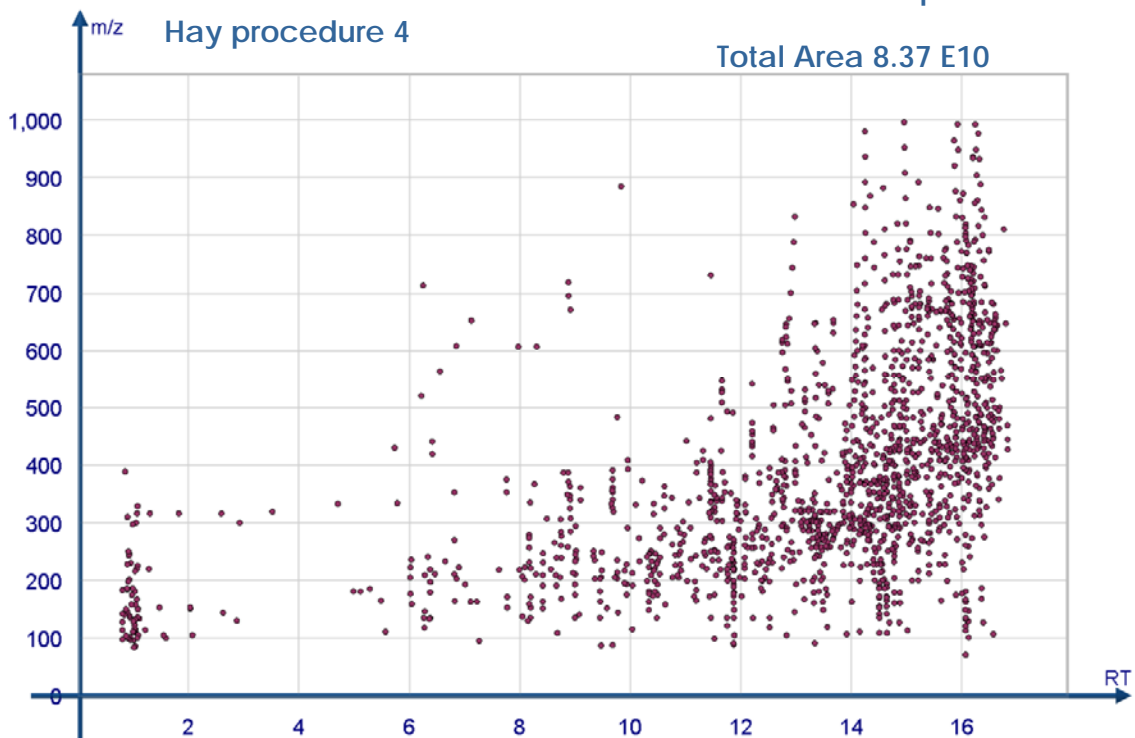
2658 Matrix compounds



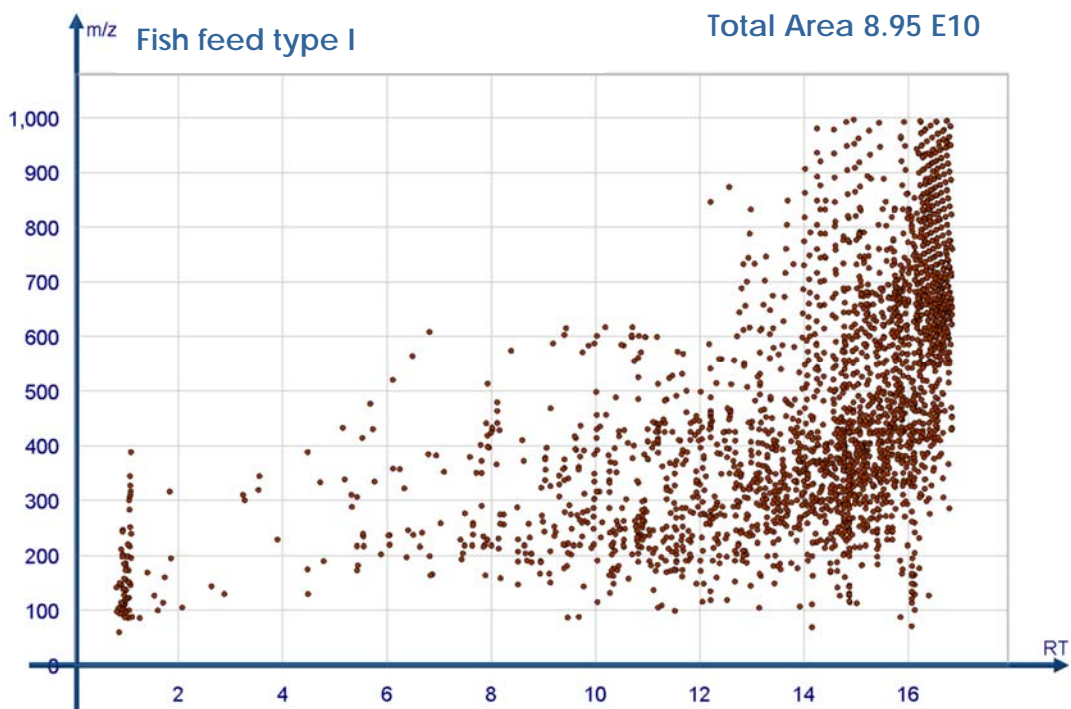
2889 Matrix compounds



1639 Matrix compounds



2805 Matrix compounds



2284 Matrix compounds

