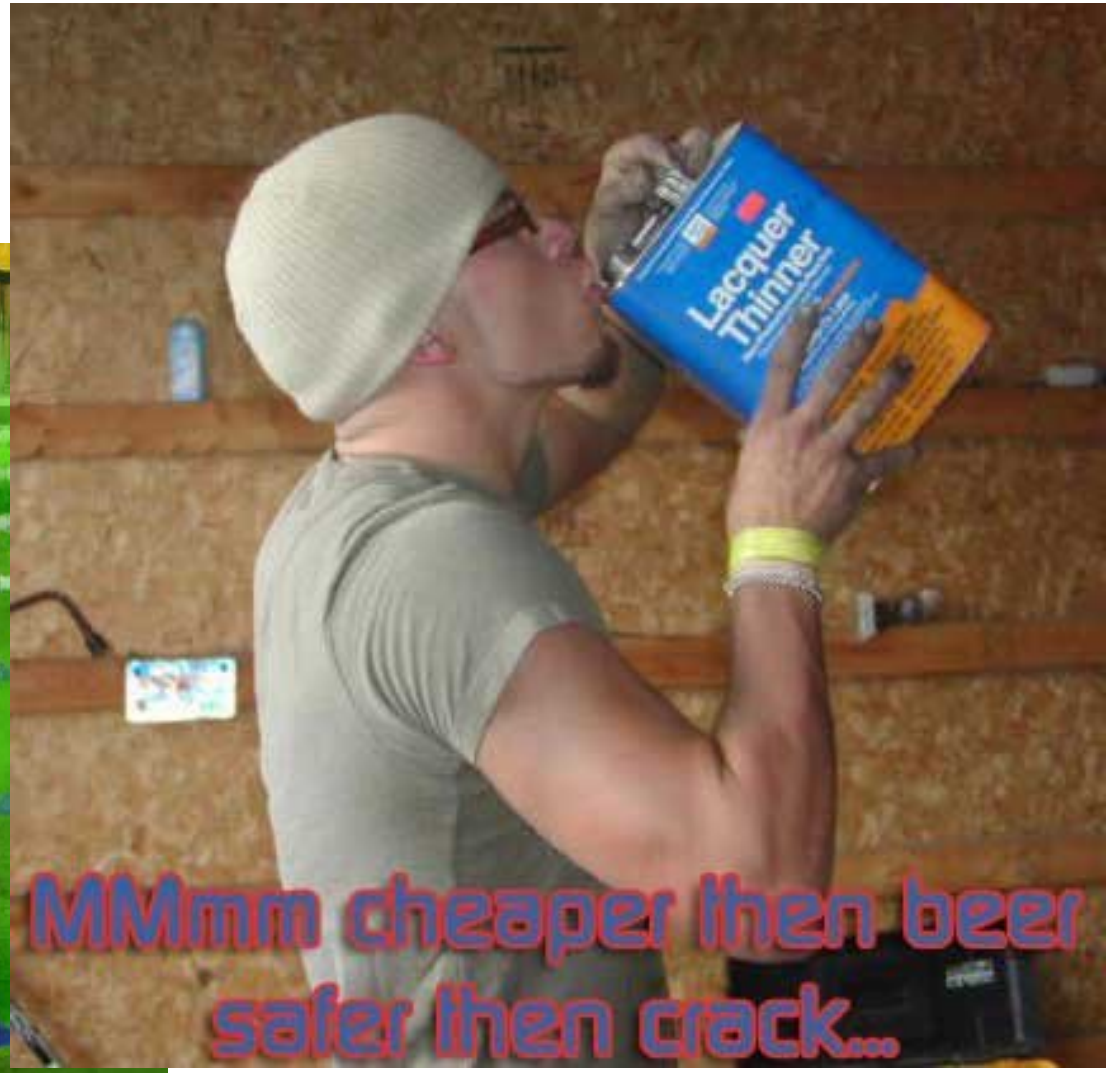
Measuring Microplastic Unknowns, When They Go Low We Can Go High

(Resolution)


TOXIC WASTE
Worth1000.com

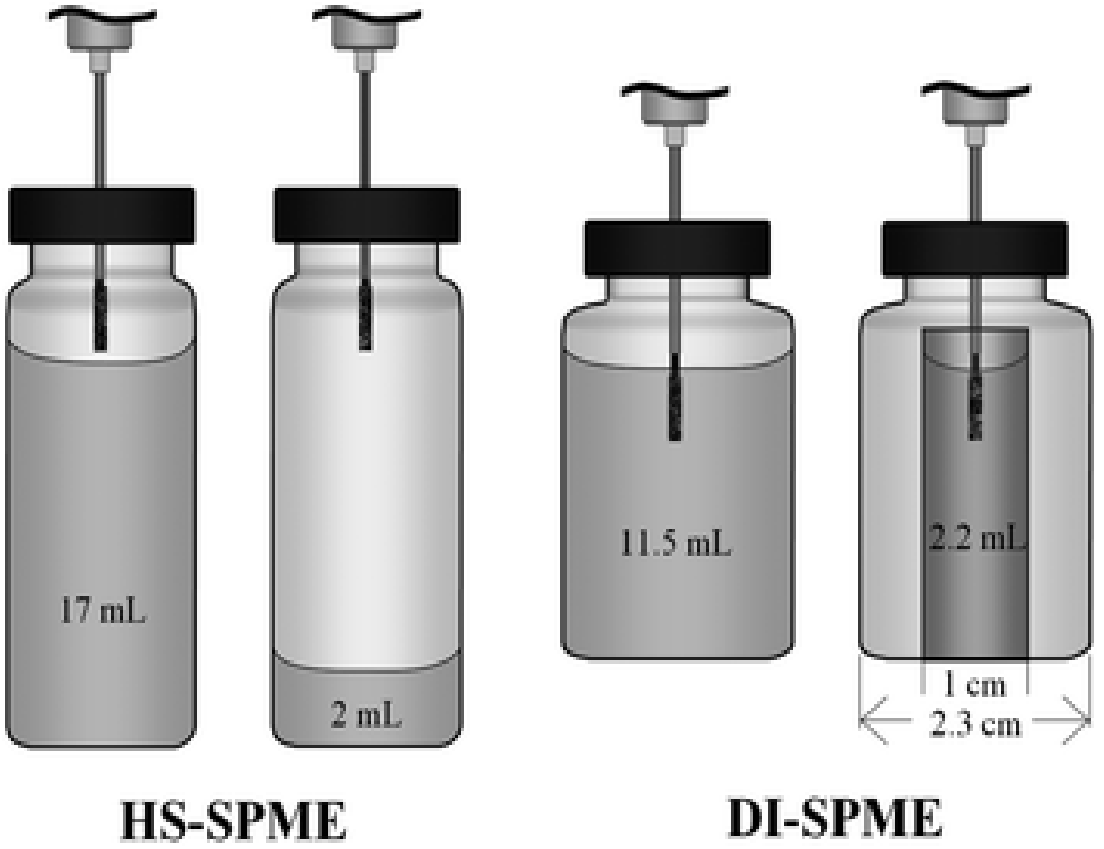

Lacquer Thinner
MMmm cheaper then beer
safer then crack...

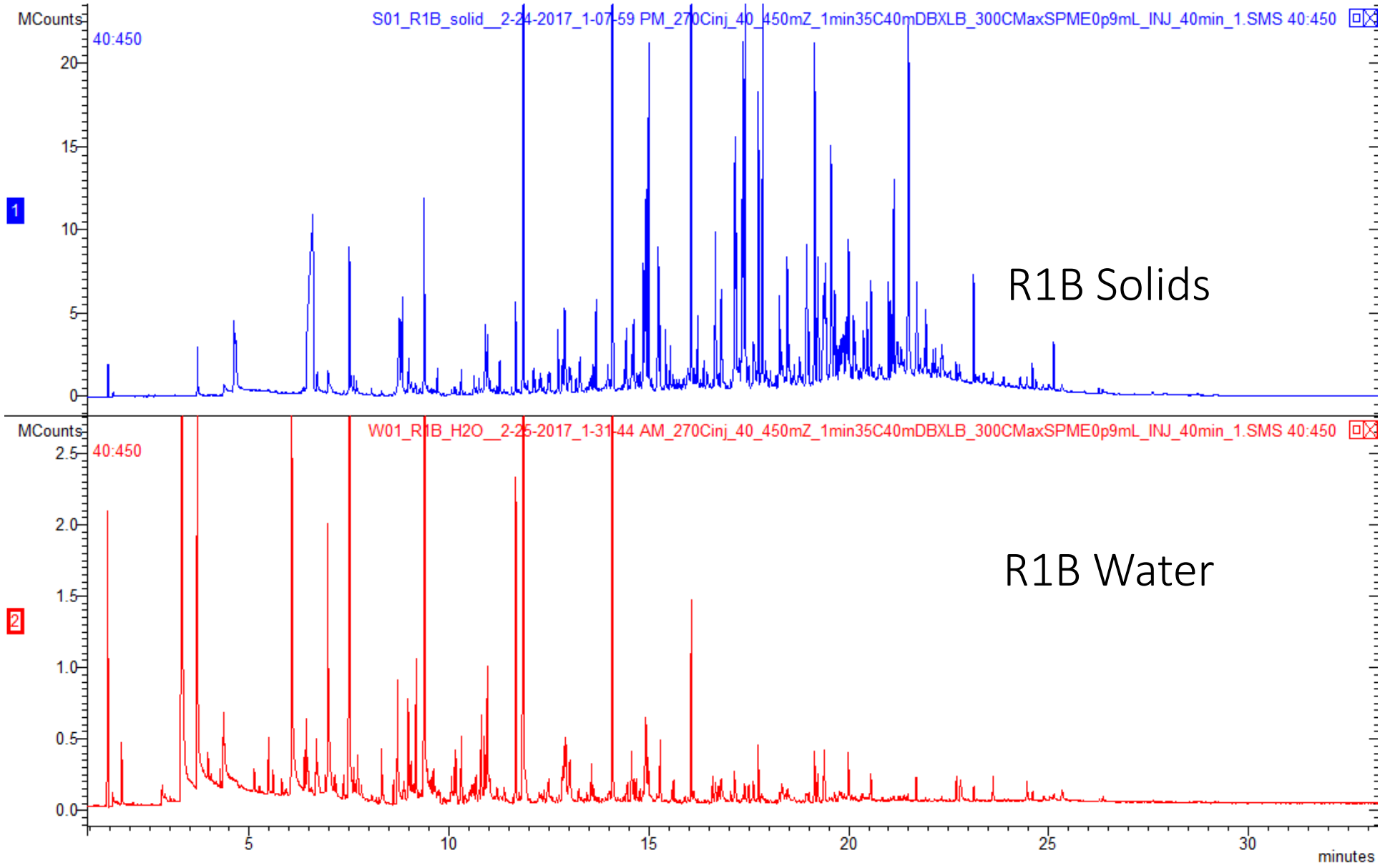
On the metals side

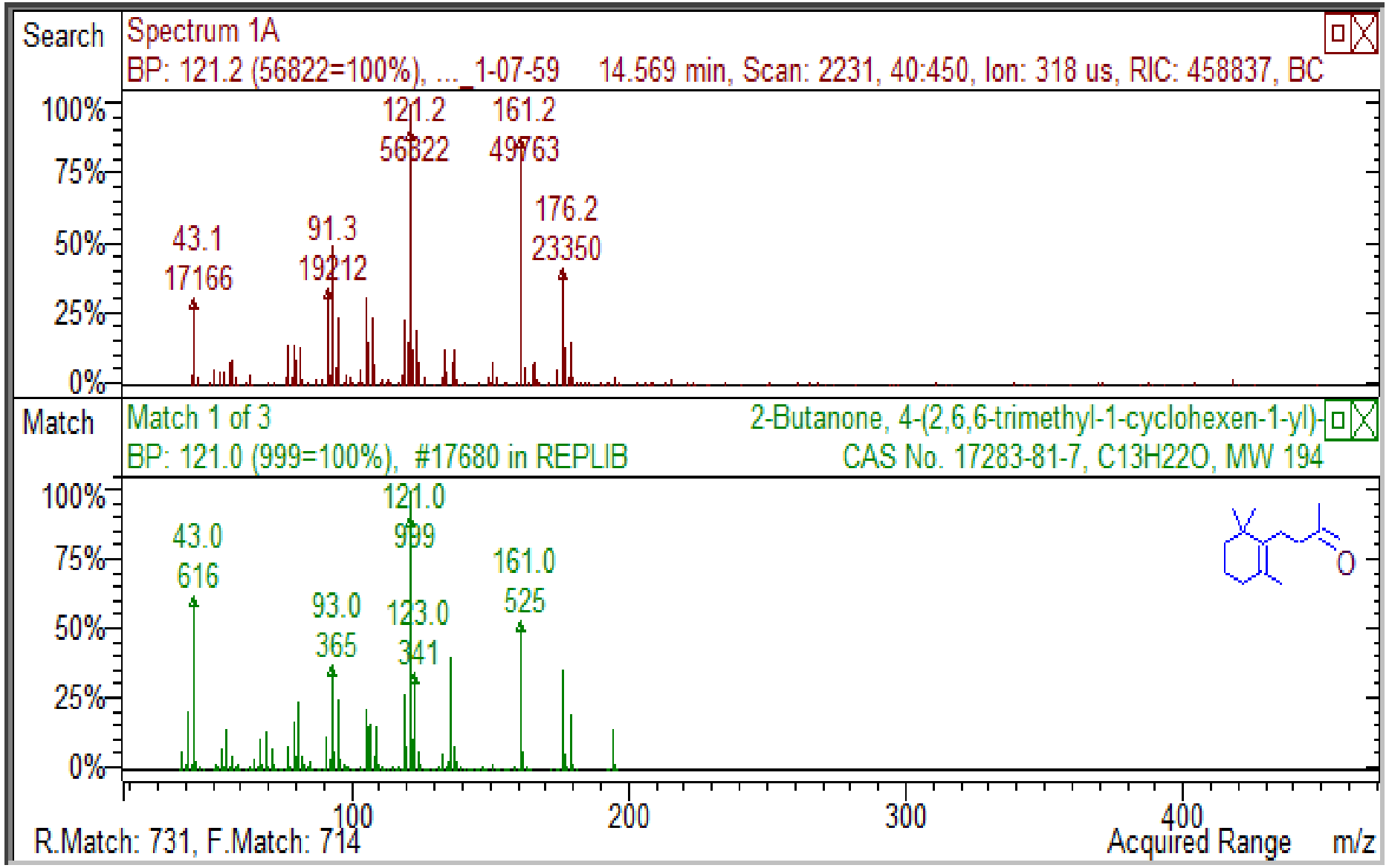
Organic analysis (GC)

Saturn 20

Solid Phase Micro Extraction

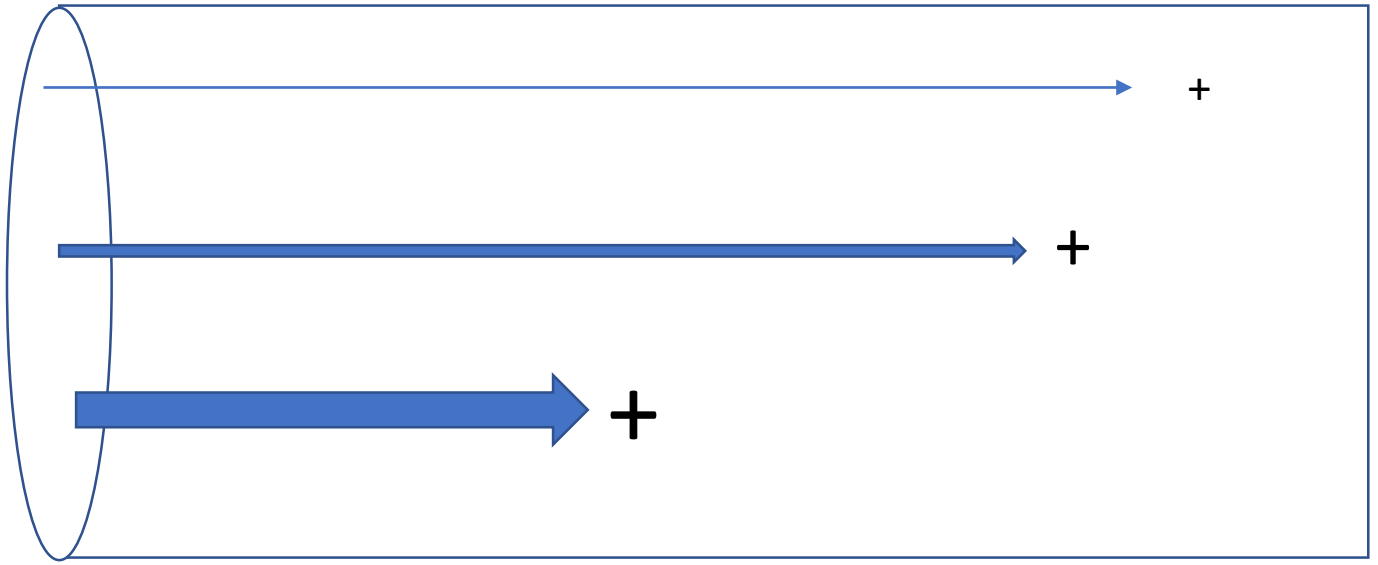



MCounts
40:450
S01_R1B_solid__2-24-2017_1-07-59 PM_270Cinj_40_450mZ_1min35C40mDBXLB_300CMaxSPME0p9mL_INJ_40min_1.SMS 40:450
1
R1B Solids
MCounts
40:450
W01_R1B_H2O__2-25-2017_1-31-44 AM_270Cinj_40_450mZ_1min35C40mDBXLB_300CMaxSPME0p9mL_INJ_40min_1.SMS 40:450
2
R1B Water
minutes


Search
Spectrum 1A
BP: 121.2 (56822=100%), ... 1-07-59 14.569 min, Scan: 2231, 40:450, Ion: 318 us, RIC: 458837, BC
100%
75%
50%
25%
0%
121.2
56822
161.2
49763
176.2
23350
91.3
19212
43.1
17166
Match
Match 1 of 3
BP: 121.0 (999=100%), #17680 in REPLIB
2-Butanone, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
CAS No. 17283-81-7, C13H22O, MW 194
121.0
999
43.0
616
161.0
525
93.0
365
123.0
341
O
100
200
300
400
Acquired Range
m/z
R.Match: 731, F.Match: 714

Organic analysis (LC)

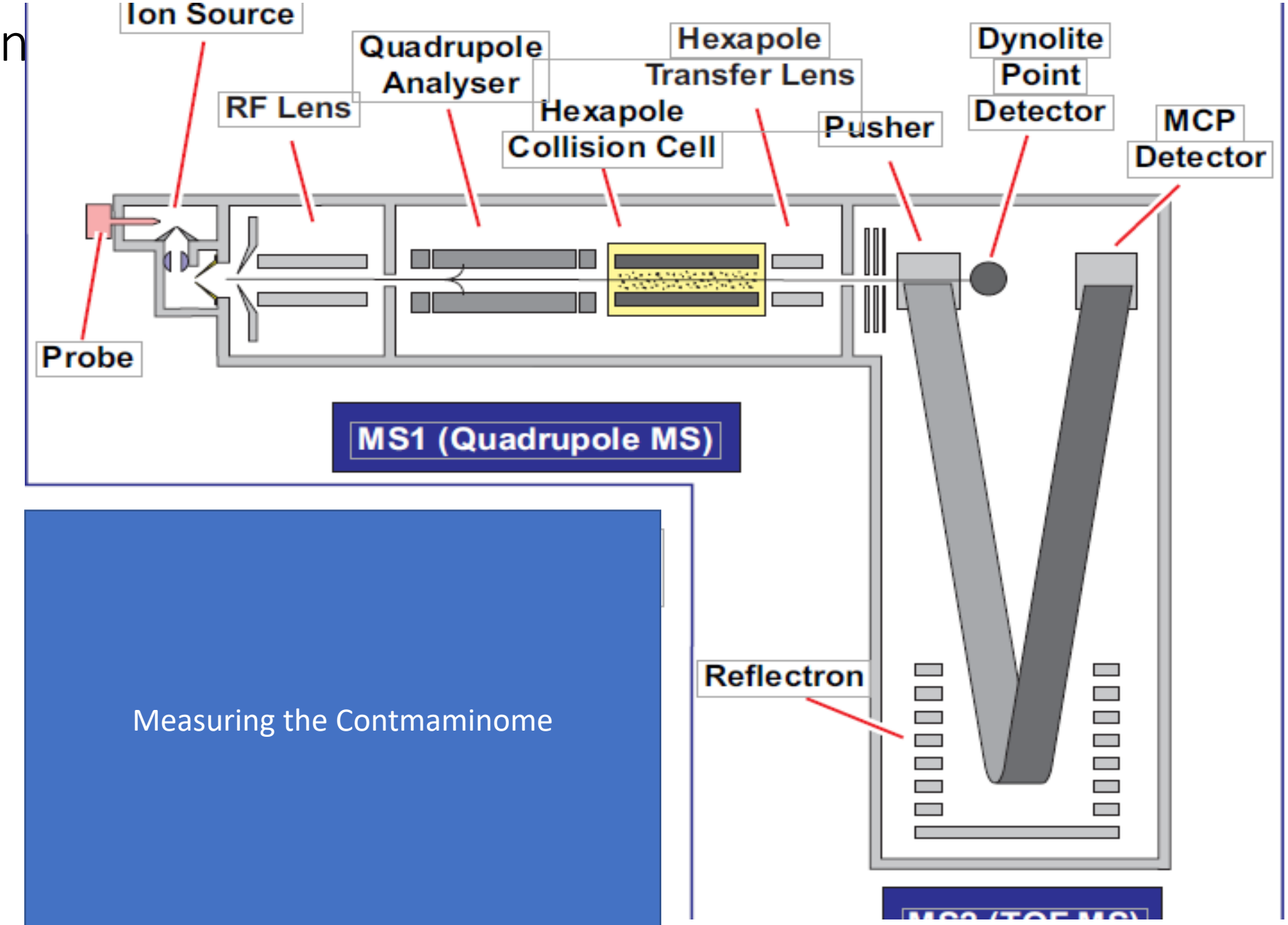
Time of Flight (ToF) Strait Flight Tube



Assume all start with the same kinetic energy

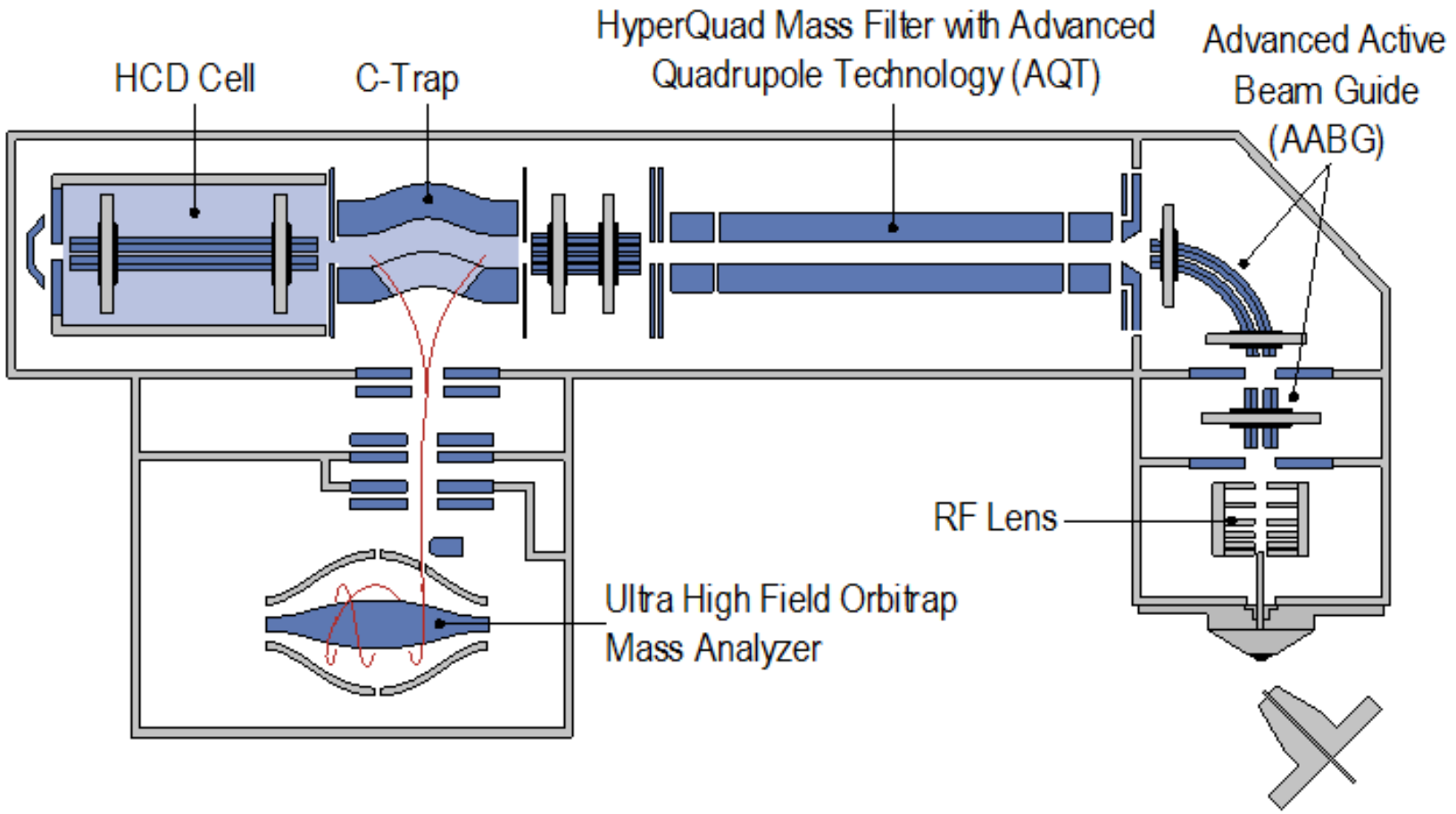
V-Configuration

Longer flight path gives better resolution as all mass to charge ratios start with the same kinetic energy



Measuring the Contmaminome

Q-Exactive HF

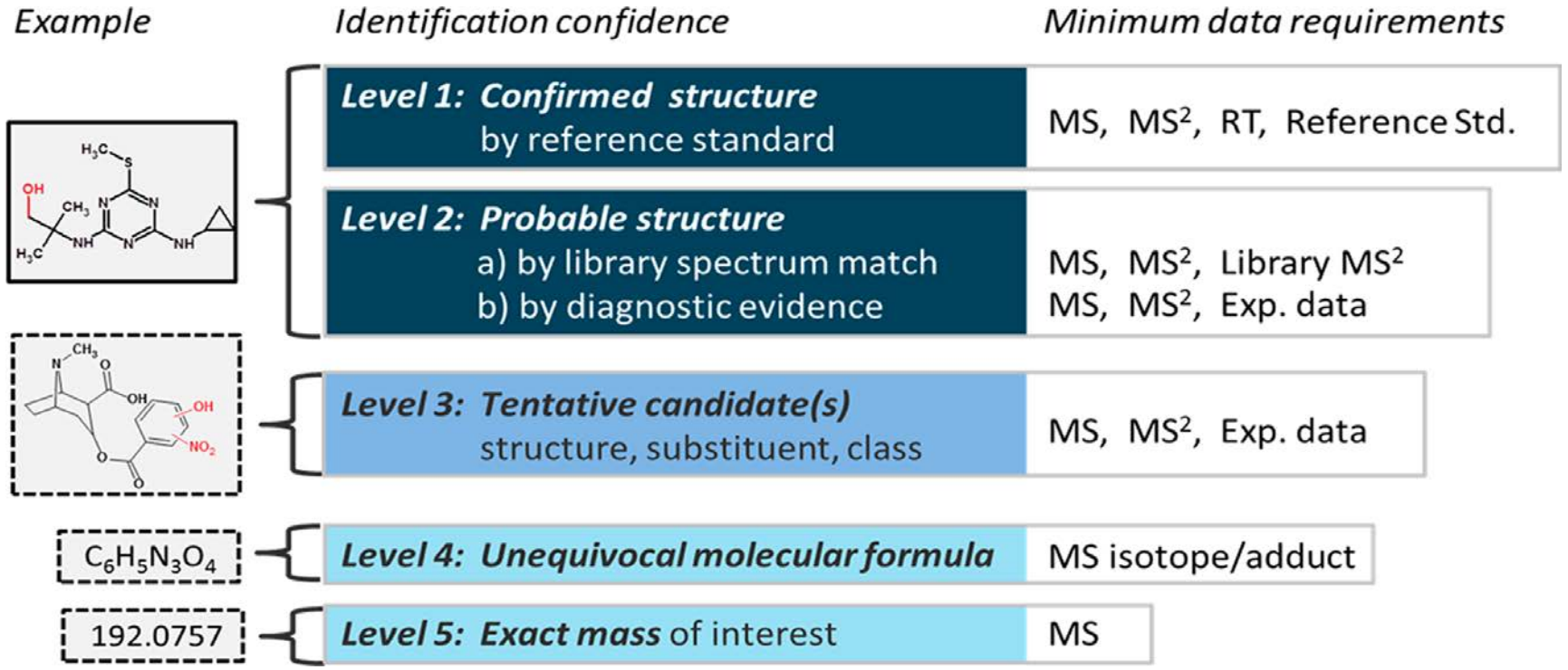


Making Sense of the Data

- Need to identify all of these unknowns
- Start with accurate mass
  - Gives you a formula weight
  - Allows you to calculate a molecular formula
  - Gets you a choice of a few to 10^5 possible isomers
- Next we need to “annotate” our spectra
  - RT
  - Fragmentation patterns
  - Ion ratios
  - “CCS”
  - Match theoretical
- Confirm with standard

Welcome to the Schymanski Scale

- Identifying Small Molecules via High Resolution Mass Spectrometry



Identifying Small Molecules via High Resolution Mass Spectrometry: Communicating Confidence
Emma L. Schymanski, Junho Jeon, Rebekka Gulde, Kathrin Fenner, Matthias Ruff, Heinz P. Singer, and Juliane Hollender, Environmental Science & Technology 2014 48 (4), 2097-2098 .

Conclusion (My Predictions for the Future)

- Identification of unknown will continue to migrate from library search only to accurate mass
- SPME will become more widely utilized
- Libraries are increasing, especially on the LC/MS side
- Identification protocols are using the “metabolomic” approaches
- Schymanski scale or similar will become the standard for assigning confidence to an unknown identification
- *Ion mobility*

Thanks to the people doing the work