

RAISING THE IDENTIFICATION CONFIDENCE IN NON-TARGET ANALYSIS OF HOUSE DUST BY COMBINING CLASSIC AND SOFT EI GC-HRMS

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AIM

To evaluate **Classic and Low Energy “Soft” EI**
combined with **HRMS GC/Q-TOF** to identify
organic **contaminants in complex house dust**



BACKGROUND

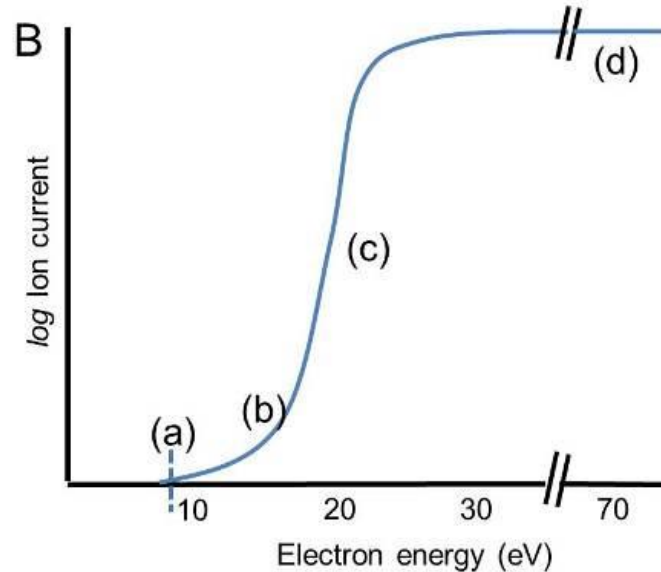
- We spend most of our time indoors and are then **exposed to potentially hazardous chemicals** via inhalation of air and dust
- Most indoor environment studies target a few compounds and the overall **combined exposure is largely unknown**
- **Non-target data acquisition** can expand our knowledge e.g. using **electron ionization GC-HRMS**, and **huge spectra libraries**
- **Classic EI** analysis is unfortunately often **hampered by a lack of molecular ion information** – a limitation we currently try to address

MOLECULAR IONS OR SENSITIVITY?

- a) Molecular ions starts to form
- b) Fragment ions starts to form
- c) Significant fragmentation
- d) Max ion yield

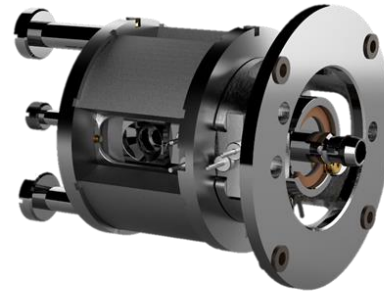
How to get molecular ions and sensitivity?

High efficiency ion source



HIGH EFFICIENCY – LOW eV EI

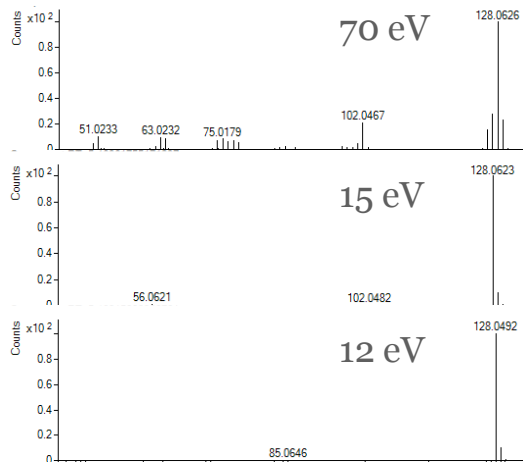
Agilent 7250
GC/Q-TOF



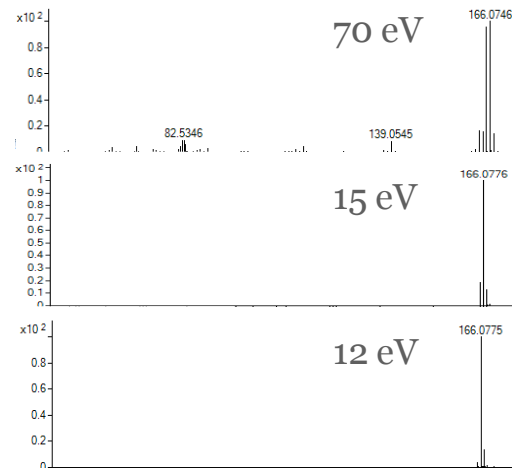
Proprietary
Low Energy
EI Source

PAH

Naphthalene

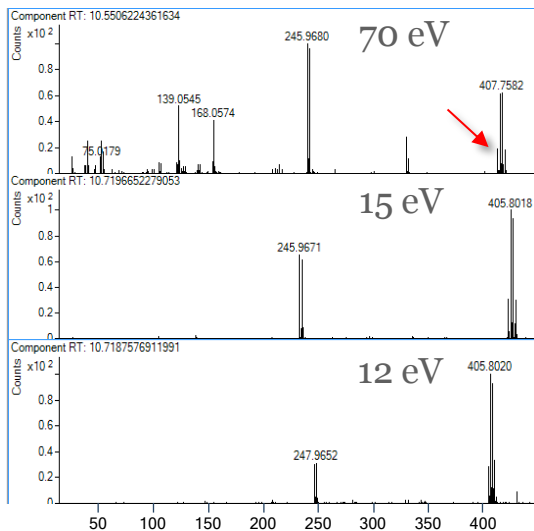


Fluroene



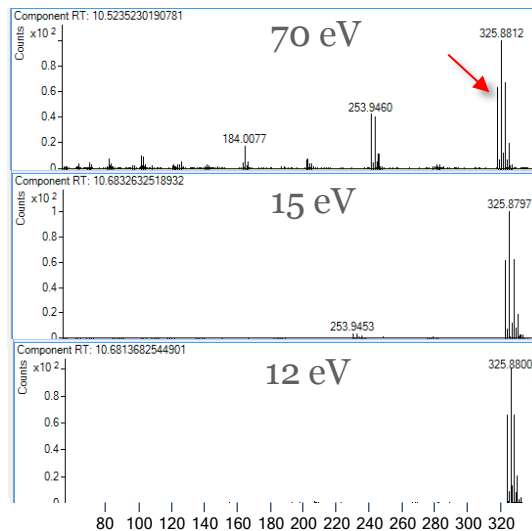
PBDE

2,4,4'-Tribromodiphenyl ether
(PBDE 28)

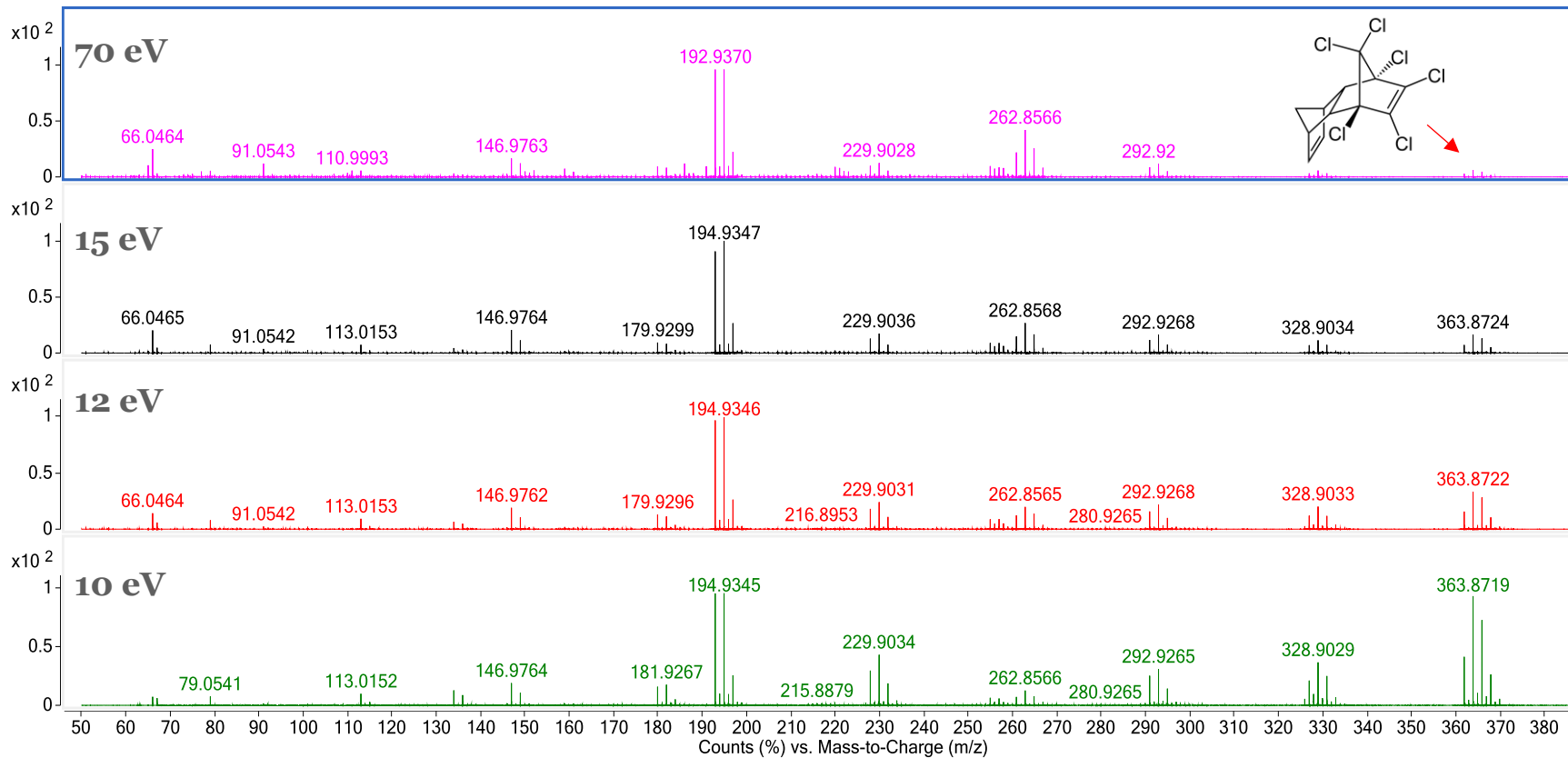


PCB

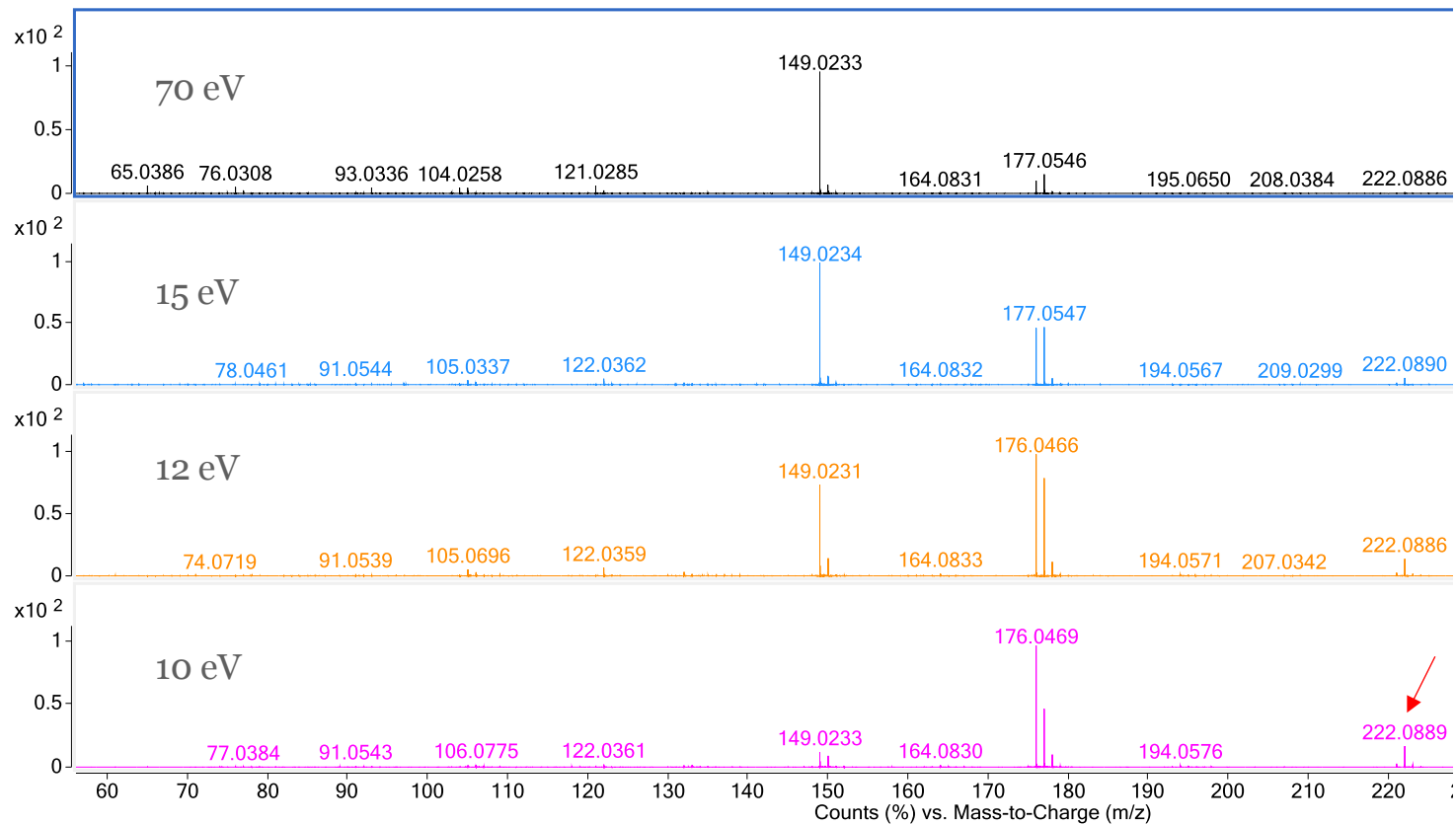
2,2',4,5,5'-Pentachlorobiphenyl
(PCB 101)



ISODRIN (pesticide)



Diethyl Phthalate



EXPERIMENTAL

- Sample: NIST 2585 reference dust
- Extraction: Ultra-sonication with dichloromethane
- GC: DB-5MS; 60 m, 0.25 mm, 0.25 μm film
- MS
Agilent 7250 GC/Q-TOF, high efficiency (EI) ion source
Full scan profile data (>25,000 FWHM), 5-10 Hz
Classic EI at 70 eV and “Soft-EI” at 10 -15 eV
- Evaluation: Masshunter Unknown Analysis, incl. SureMass

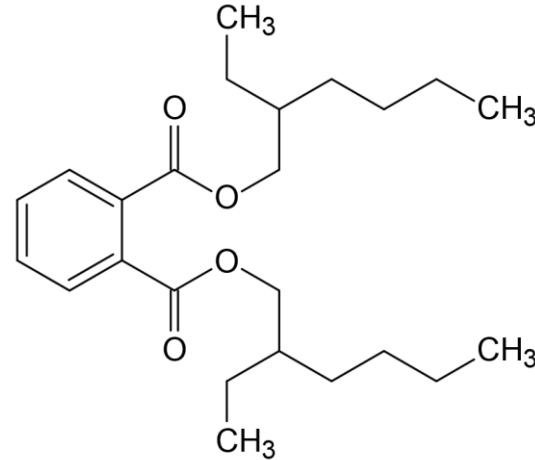
PRINCIPLE

To use **Classic EI** and library searching to obtain the **tentative structures**

To use **Soft-EI** increase the proportion of **molecular ions** or **high molecular weight fragment ions**

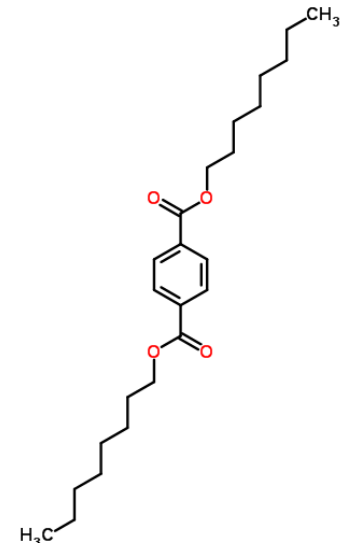
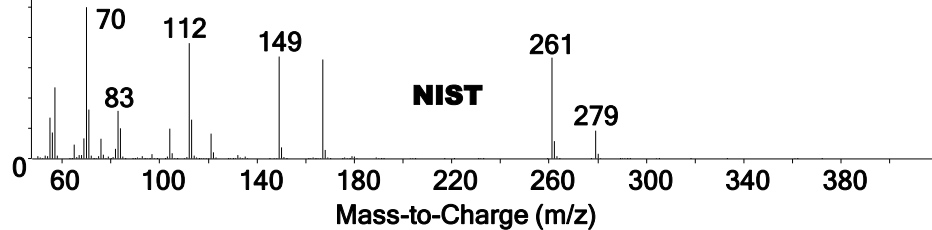
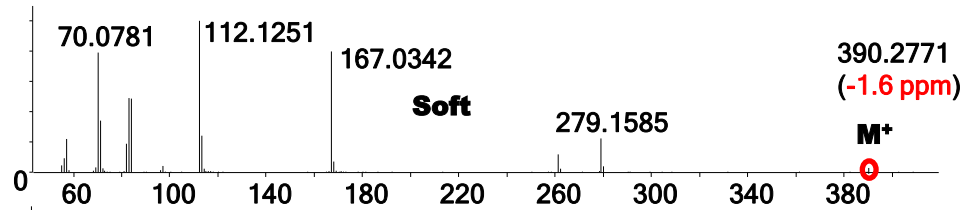
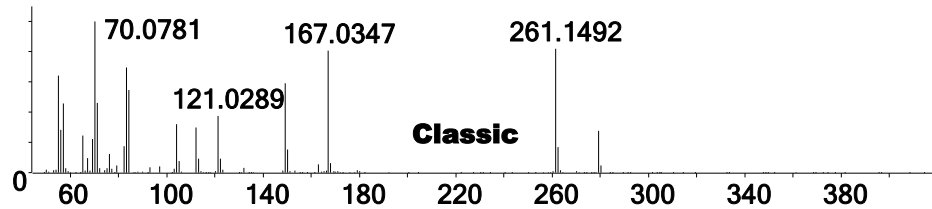
PLASTICIZERS IN DUST

- **DEHP** phased out
- What is used instead?
- Other plasticizers?

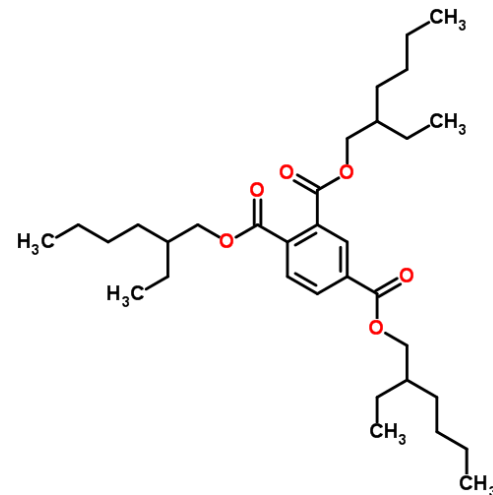
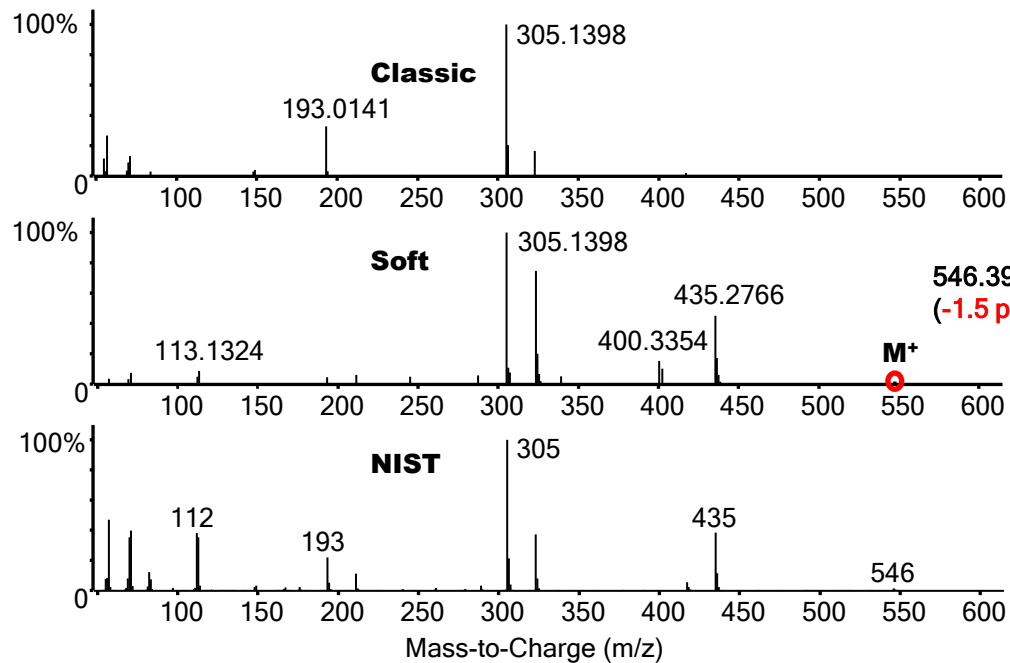


- *Focus on late eluting compounds*

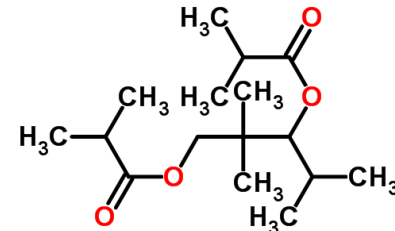
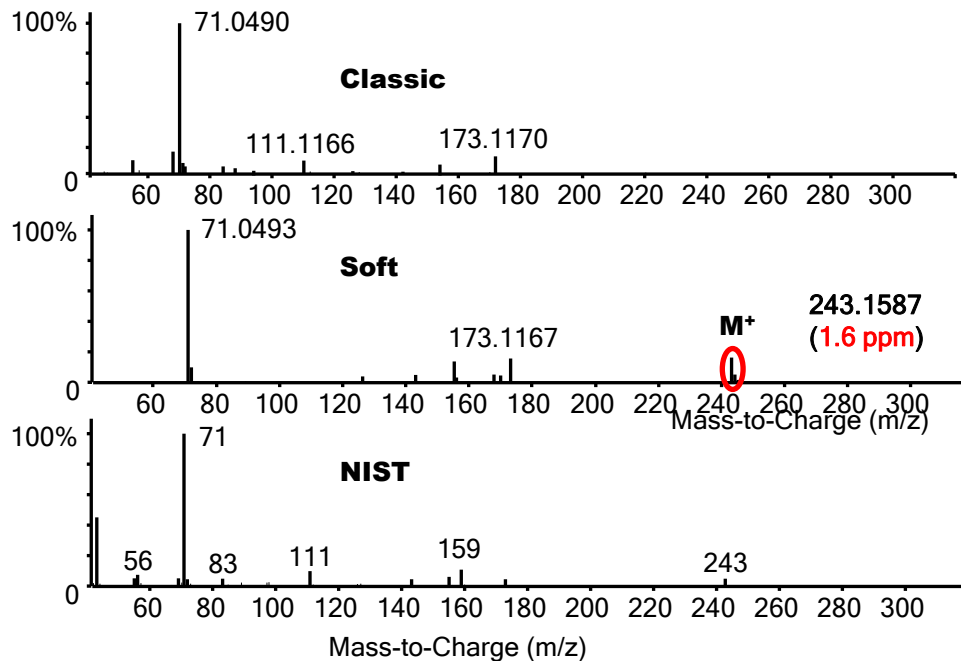
DIOCTYL TEREPHTHALATE (DOTP)



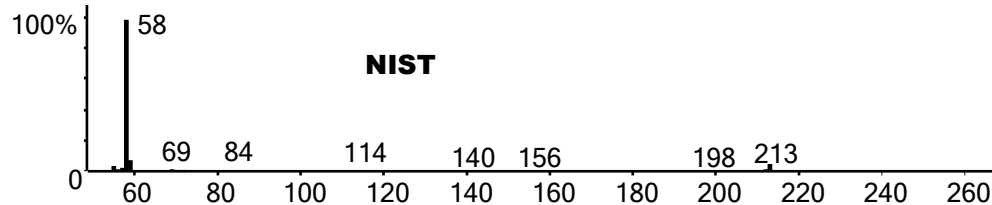
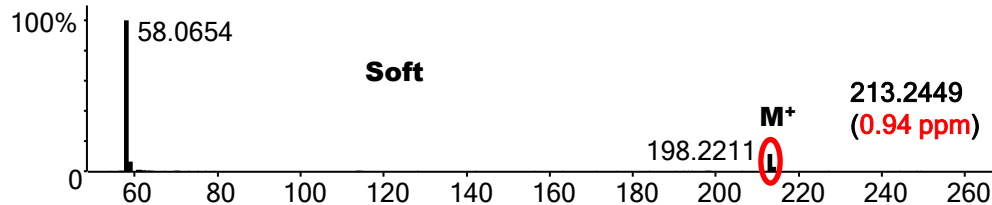
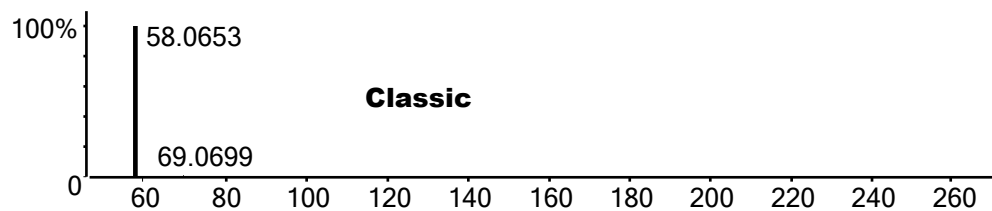
TRI(2-ETHYLHEXYL)TRIMELLITATE (TOTM)



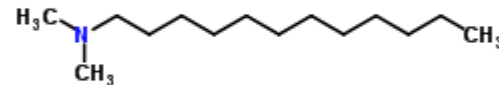
TRIMETHYL PENTANYL DIISOBUTYRATE (TXIB)



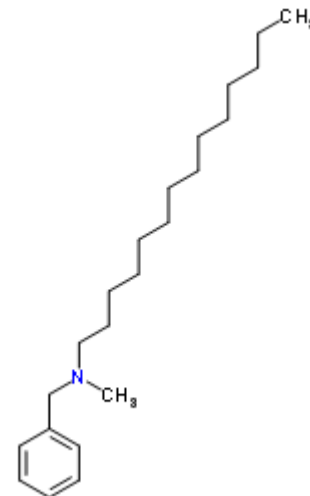
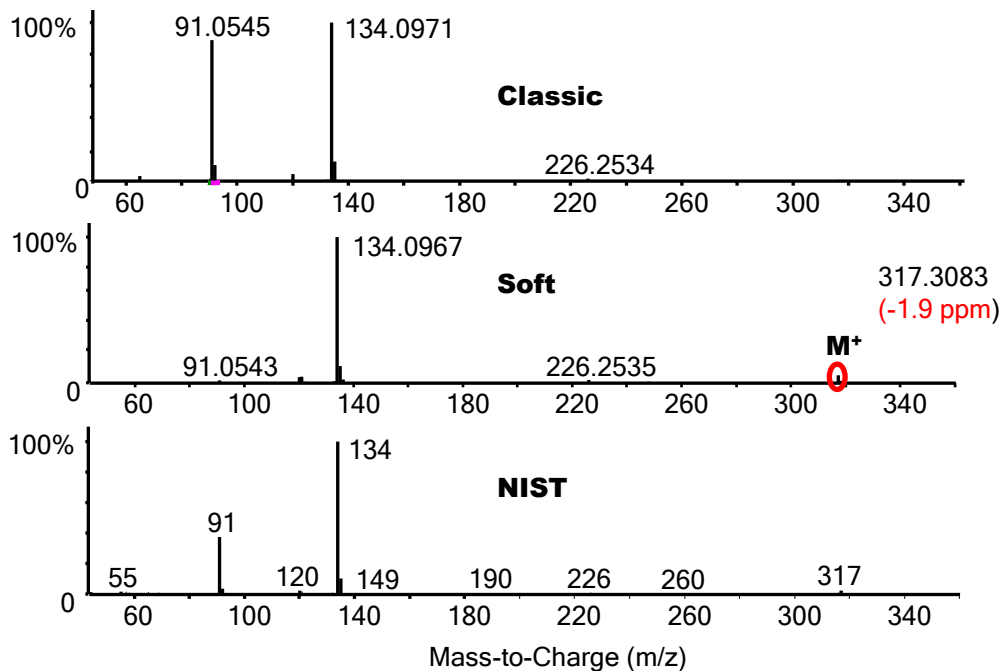
***N,N*-DIMETHYL-*N*-DODECANAMINE (C₁₂-DM-A)**



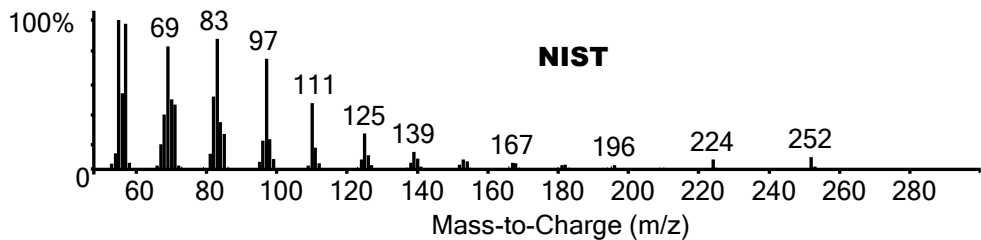
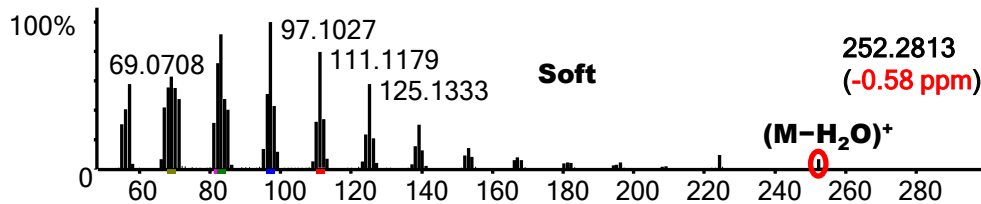
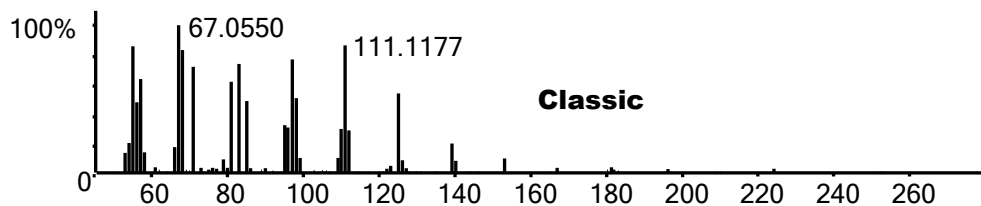
Mass-to-Charge (m/z)



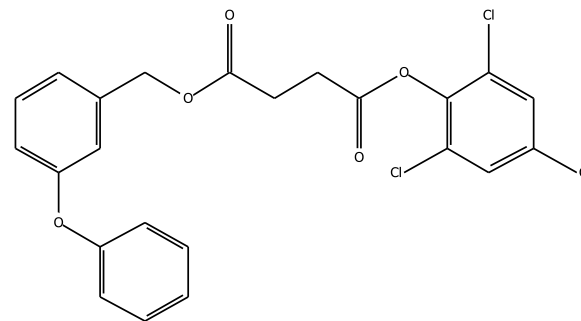
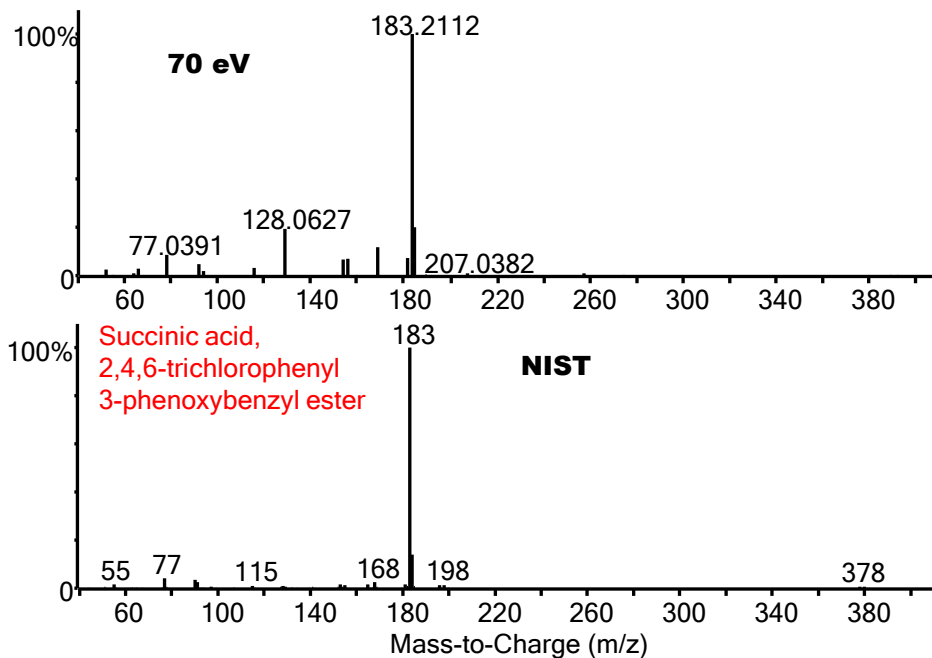
N-METHYL-N-BENZYL-TETRADECANAMINE (C₁₄-MBZ-A)



1-OCTADECANOL (C₁₈-OH)

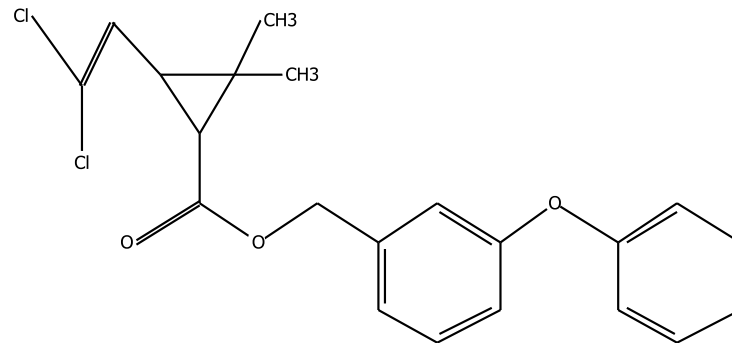
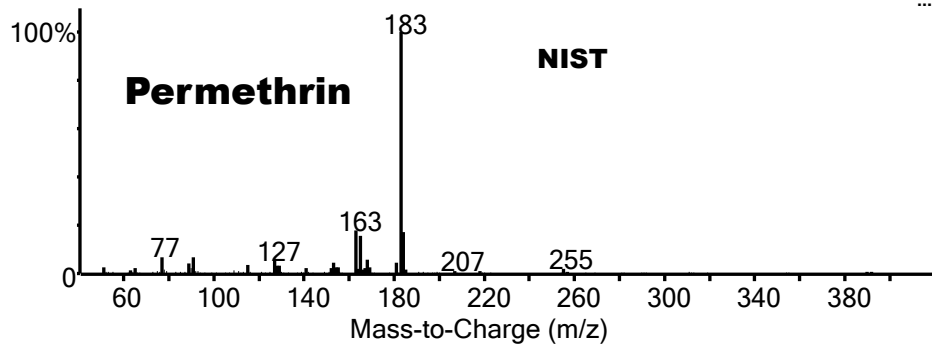
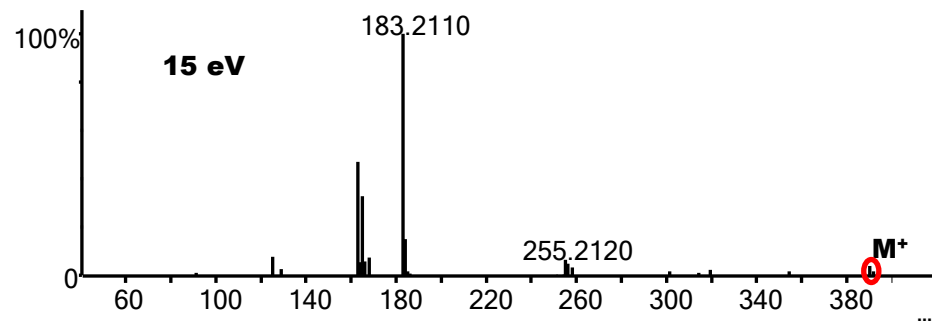


SUCCINIC ACID, 2,4,6-TRICHLOROPHENYL 3-PHENOXYBENZYL ESTER



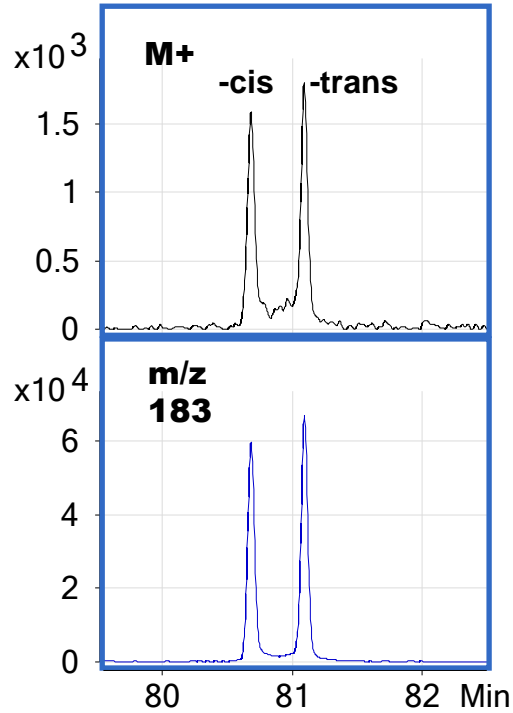
No hit in ChemSpider !?

PERMETHRIN?



PERMETHRIN !

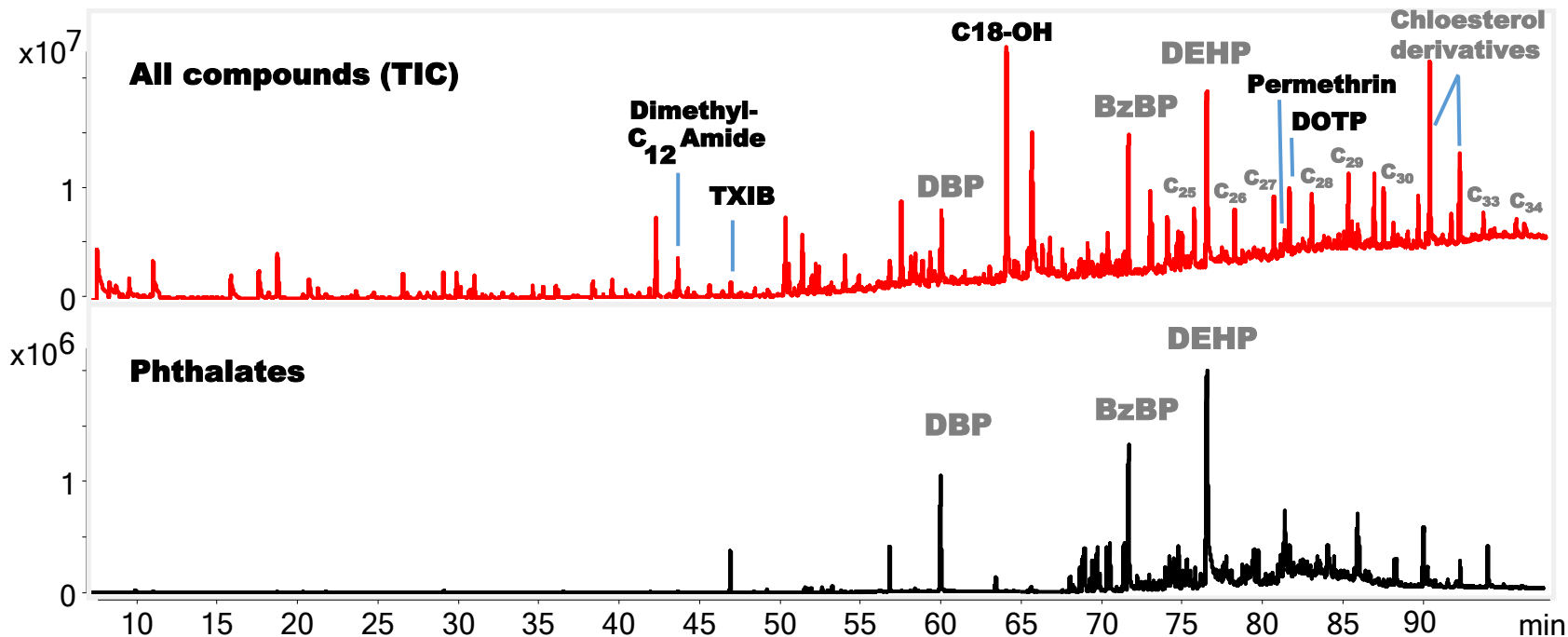
CORRECTION OF MISSASSIGNMENT!



LOWER BACKGROUND

- **Softer ionization**
- **Less fragmentation, less column bleed ions**
- **Easier deconvolution - Cleaner spectrum**

SUMMARY OF NIST DUST



CONCLUSIONS

- **Soft EI** compliments classic EI and **raises the identification confidence**
- **Enhanced molecular ion abundance = molecular ion mass verification**
- **Several DEHP substitutes were identified** by combined soft and classic EI
- **Soft EI reduce the risk of miss-assignments**

