Comparison of collision cross section (CCS)-m/z trendlines of perfluoroalkyl carboxylic acid dimers between Trapped, Traveling Wave and Drift Tube ion mobility spectrometry.

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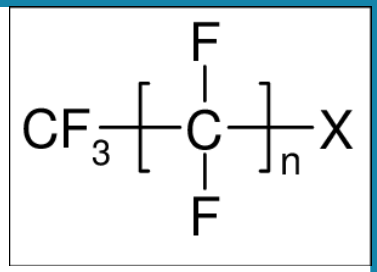
[2] Toxicological Centre, University of Antwerp, 2610 Antwerp, Belgium

ISIMS 2023

PFAS: Persepectives offered by IMS

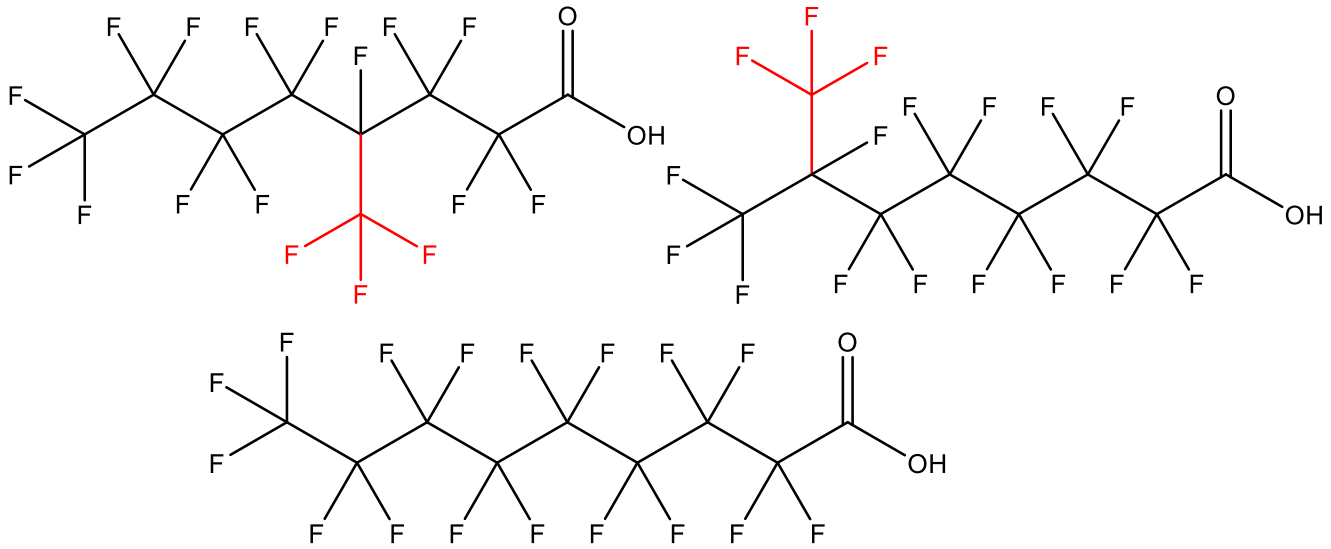


PFASs (per- and polyfluorinated substances): ± 5000 compounds

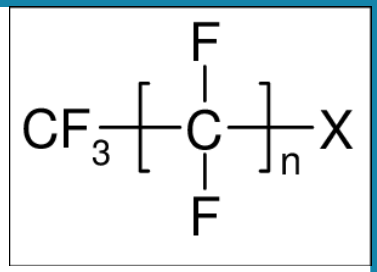
⇒ Need for large-scale suspect and non-targeted screening approaches

Usually performed by LC-HRMS but some limitations:

- Separation of isomers



PFAS: Persepectives offered by IMS

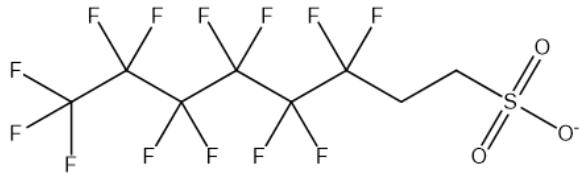


PFASs (per- and polyfluorinated substances): ± 5000 compounds

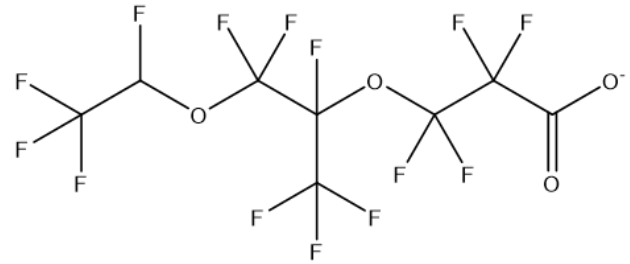
⇒ Need for large-scale suspect and non-targeted screening approaches

Usually performed by LC-HRMS but some limitations, among current challenges:

- Separation of isomers
- Identification of isobars

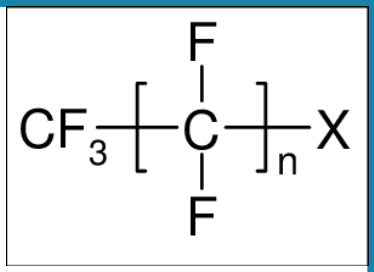


6:2 FTS
m/z 426.9674



Hydro-EVE
m/z 426.9651

PFAS: Persepectives offered by IMS



PFASs (per- and polyfluorinated substances): ± 5000 compounds

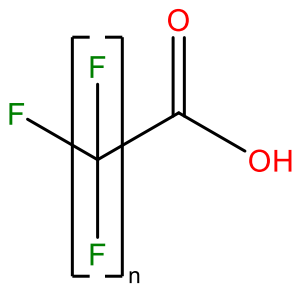
⇒ Need for large-scale suspect and non-targeted screening approaches

Usually performed by LC-HRMS but some limitations:

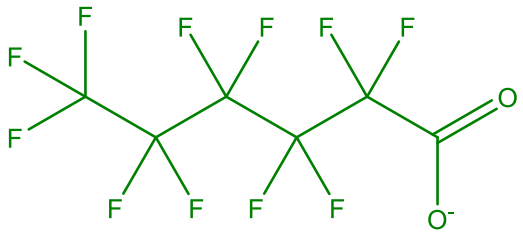
- Separation of isomers
- Identification of isobars

⇒ Ion mobility spectrometry can be valuable

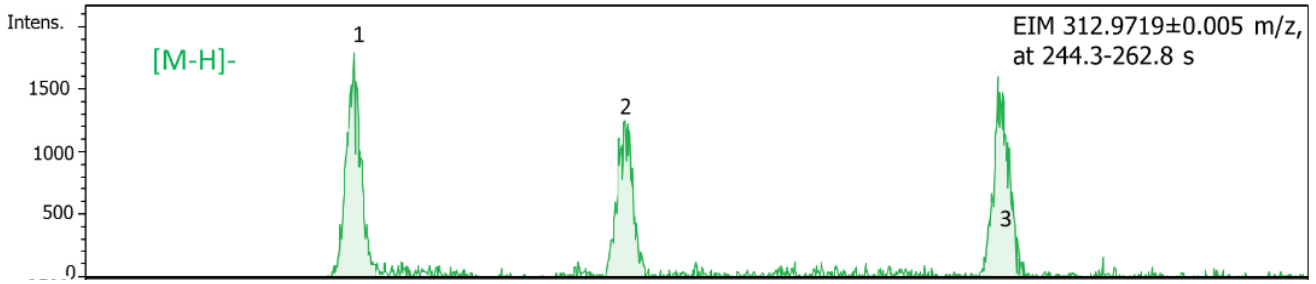
Analysis of PFCA in LC-TIMS-TOF



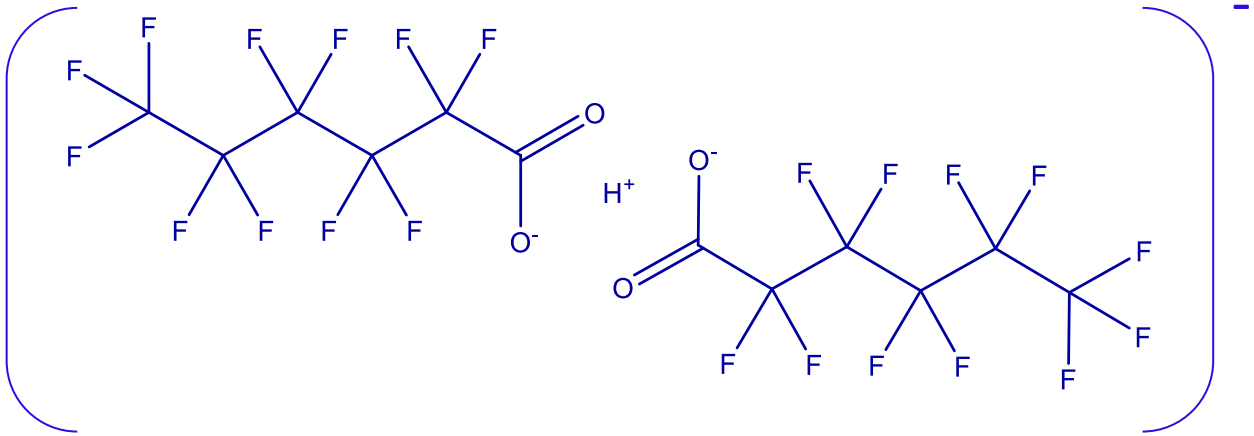
Perfluoroalkyl carboxilic acids (PFCAs)



$1/K_0$ ($\propto$CCS)

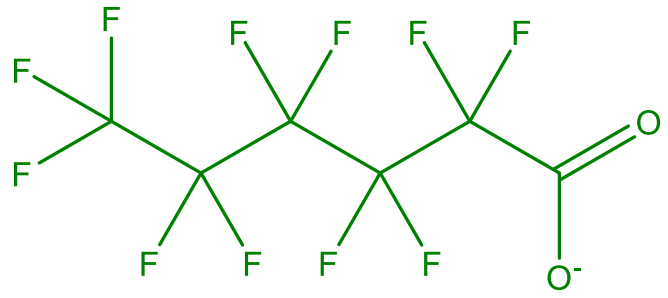


$[2M-H]^-$

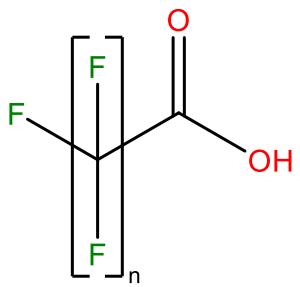


-M

$[M-H]^-$



Analysis of PFCA in LC-TIMS-TOF



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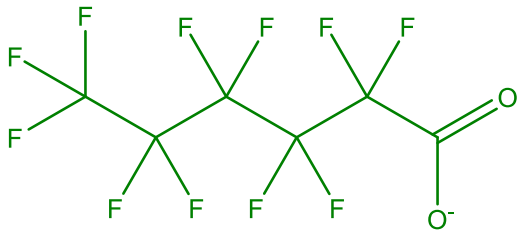

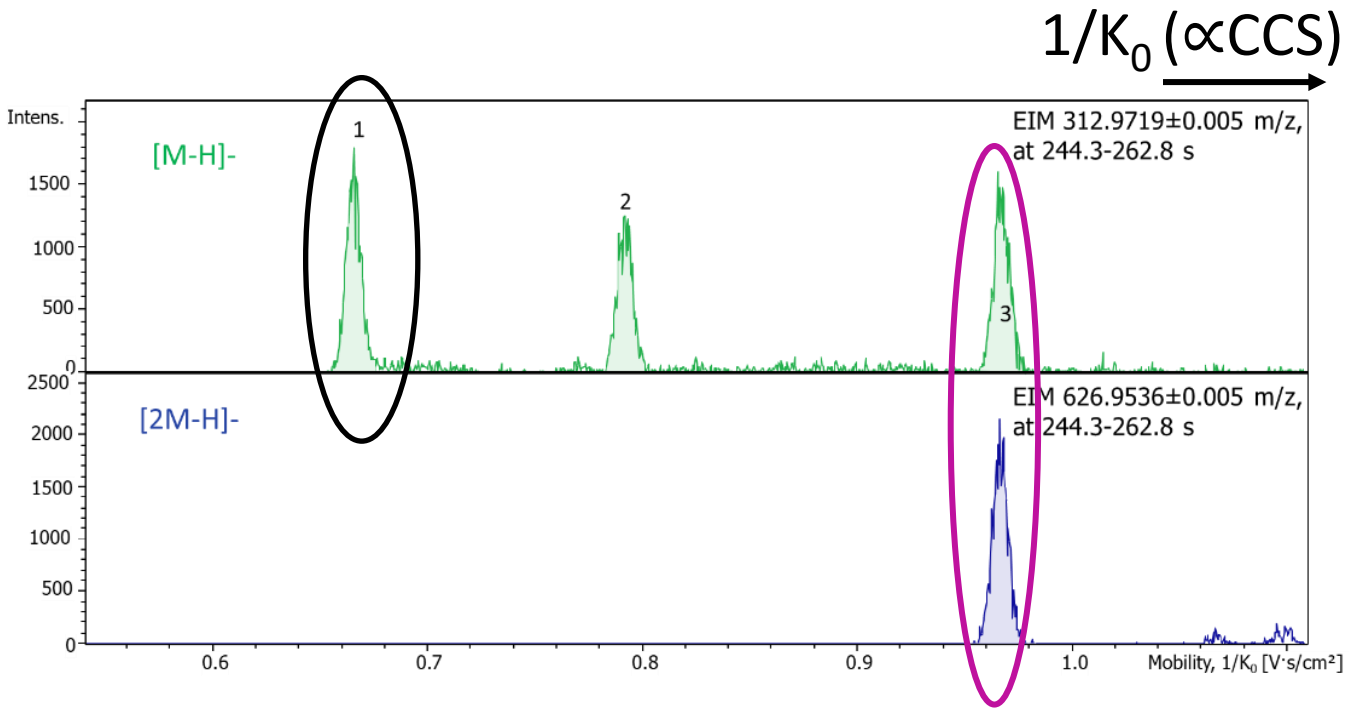

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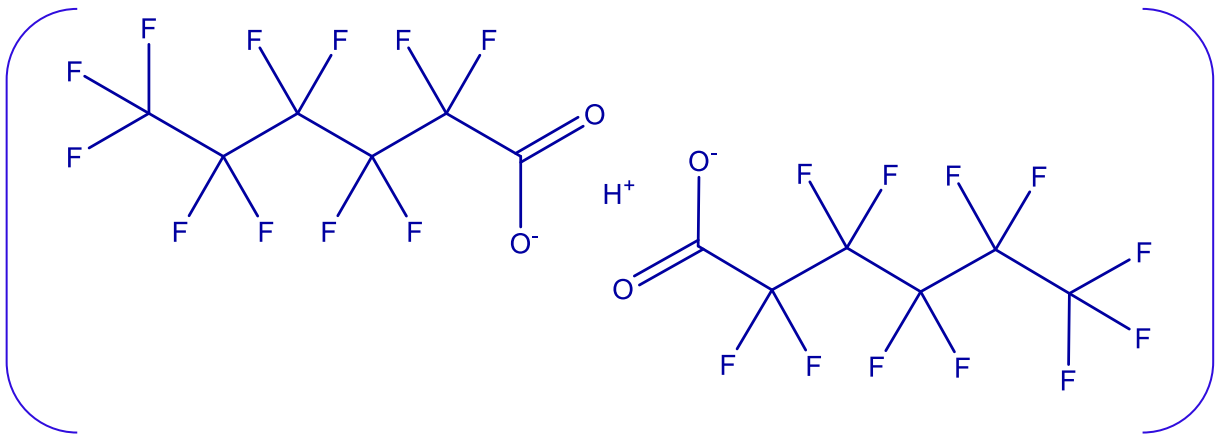
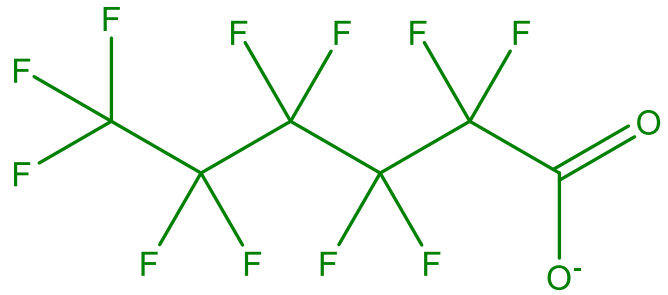


-M

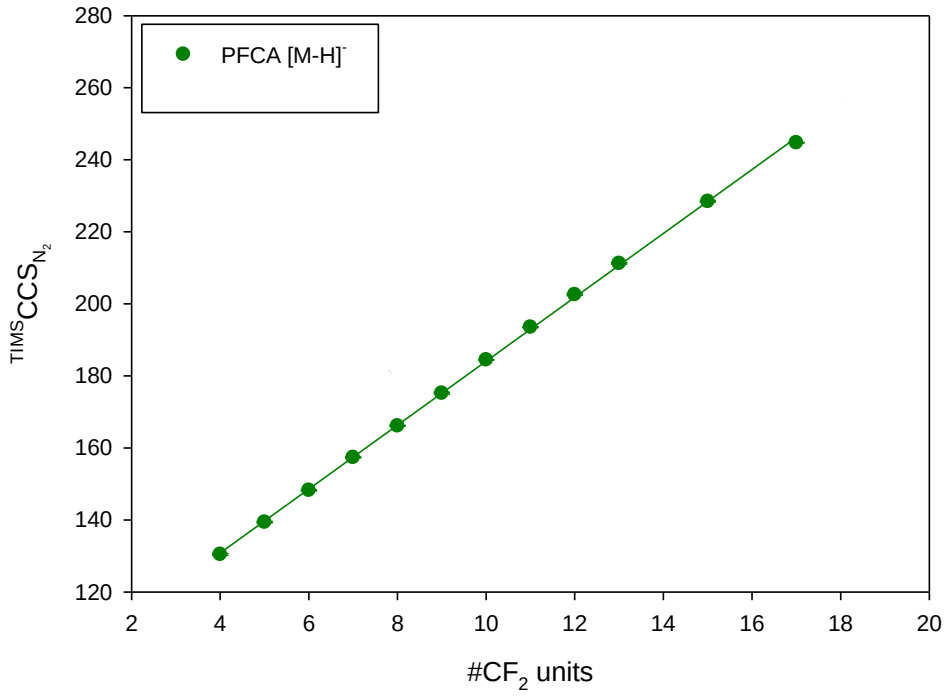
[M-H]$^-$



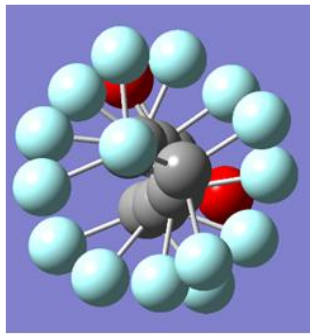
CCS-#CF_2 trendlines

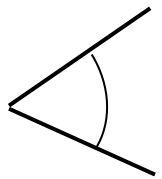
Haler, J. R. N; *et al.*; *J. Am. Soc. Mass Spectrom*. **2022**, 33 (2), 273–283.

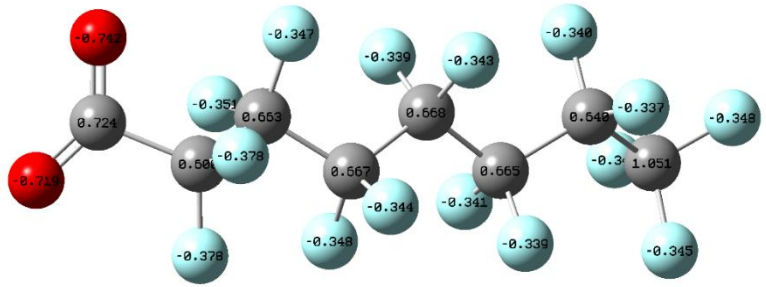
Haler, J. R. N; *et al.*; *Methods* **2018**, 144, 125–133.



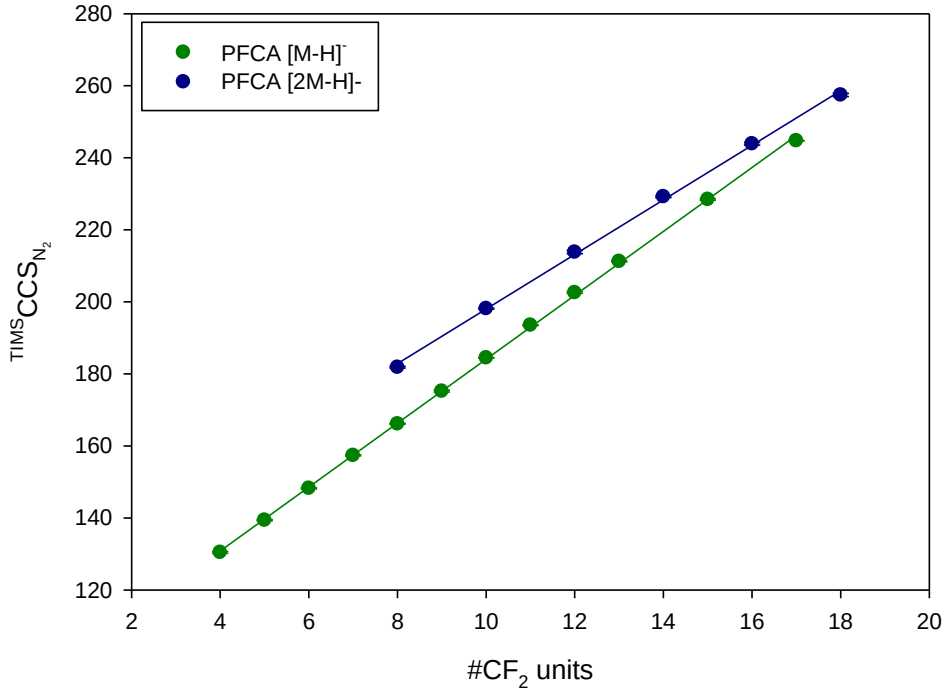
DFT CAM-B3LYP/6-31+G(d,p)







CCS-#CF_2 trendlines



Haler, J. R. N; *et al*.; *J. Am. Soc. Mass Spectrom*. **2022**, 33 (2), 273–283.

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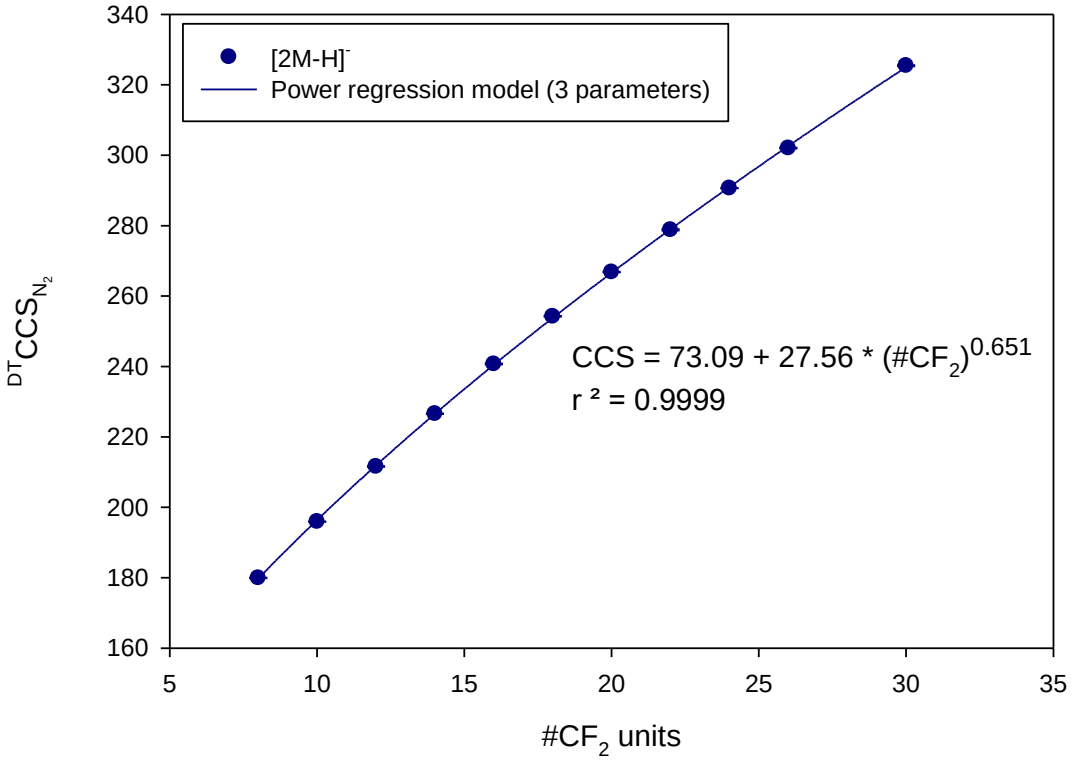
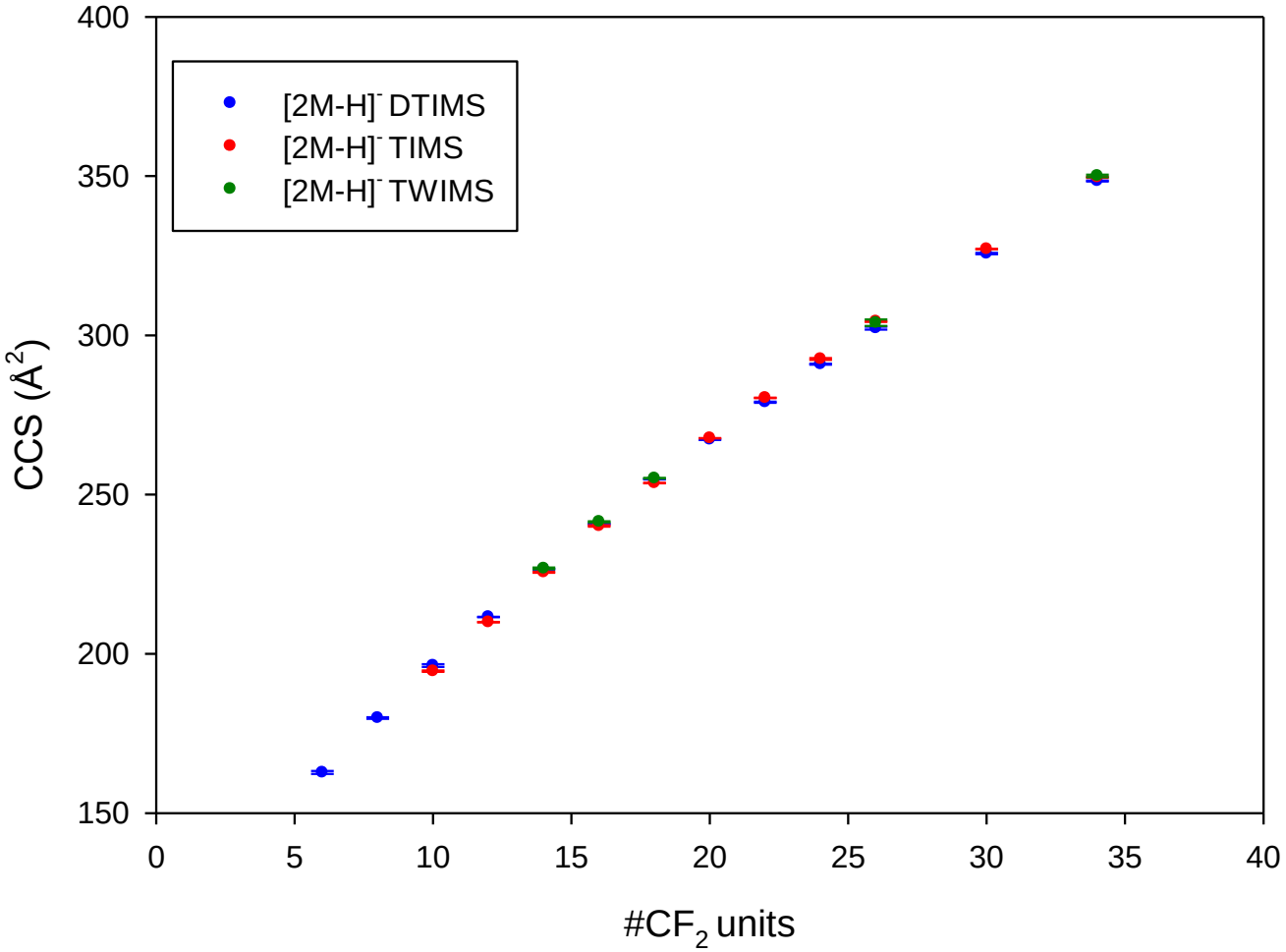


Belova, L.; et al; *Anal. Chem*. **2021**, *93* (16), 6428– 6436.

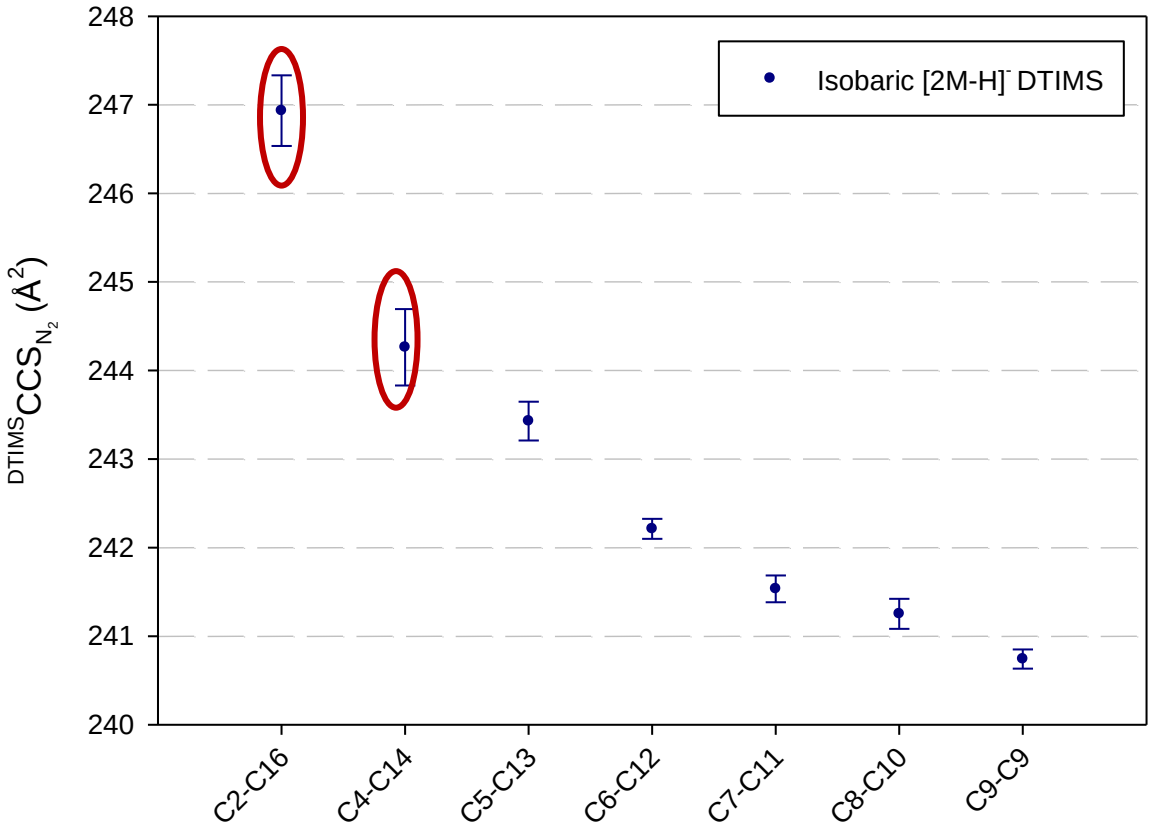
CCS-*m/z* trendlines

- Theoretical calculations

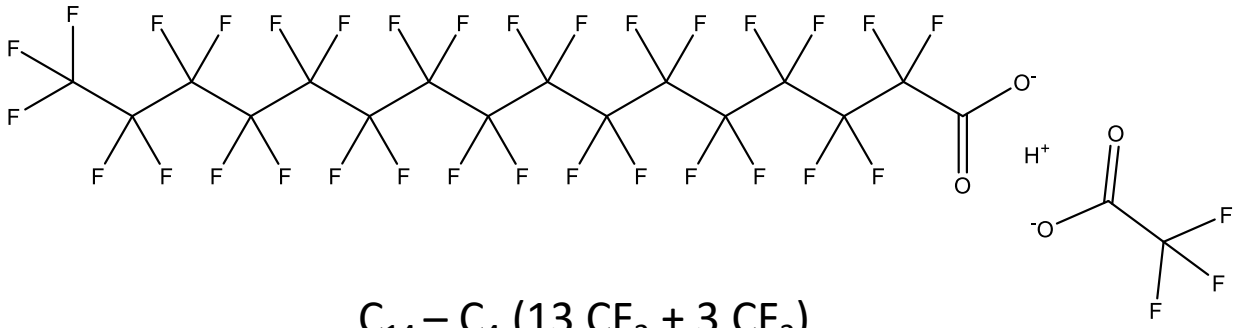
  $\Rightarrow$ Overall shape dependent of ion effective temperature?



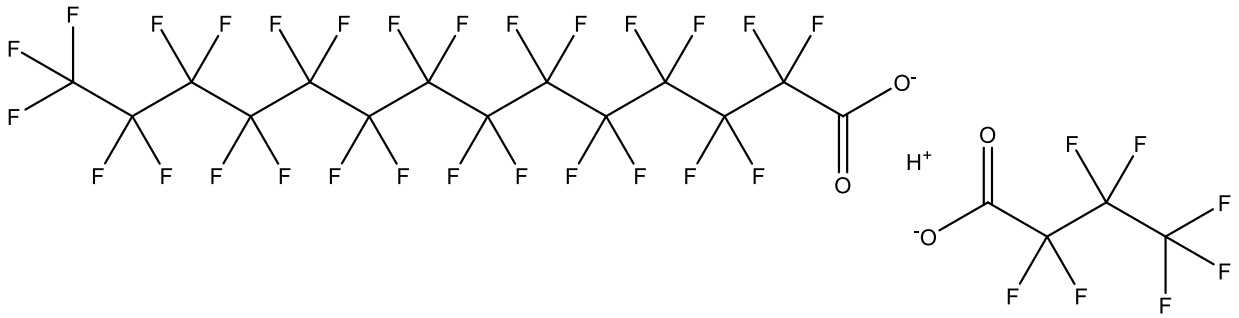
CCS of asymmetric isobaric PFCA dimers



$C_{16} - C_2$ (15 CF_2 + 1CF_2)



$C_{14} - C_4$ (13 CF_2 + 3 CF_2)



Thank you!

- Prof. Gauthier Eppe
- Dr. Far
- Prof. Edwin de Pauw
- Hugo Muller

- Prof. Adrian Covaci
- Lidia Belova

Any questions?