

REUNION DES UTILISATEURS RMN BRUKER

# Benchtop NMR: Fourier 80

## Product Updates

---

Tangi Jézéquel, Ph.D  
Ingénieur d'applications RMN  
Bruker France

## The Fourier 80 - A Family Portrait

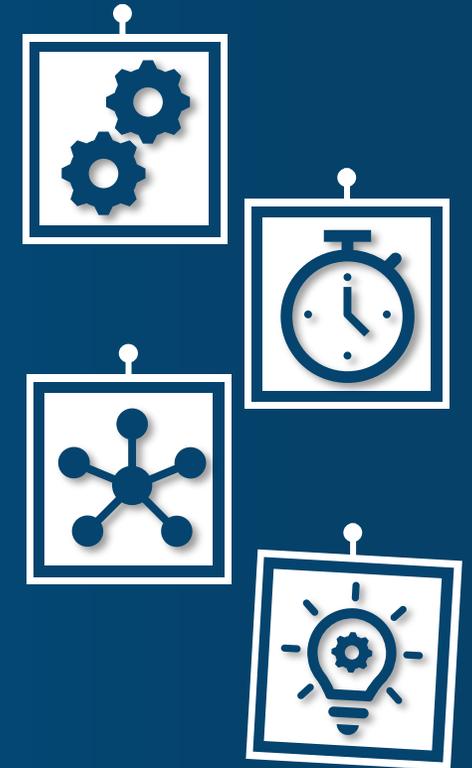
---

**01** The Workhorse  
H/C system (H S/N  $\geq$  180:1)

**02** The High Performer  
H-only system (H S/N  $\geq$  240:1)

**03** The Multi-talent  
H/C/F system (S/N-balanced)

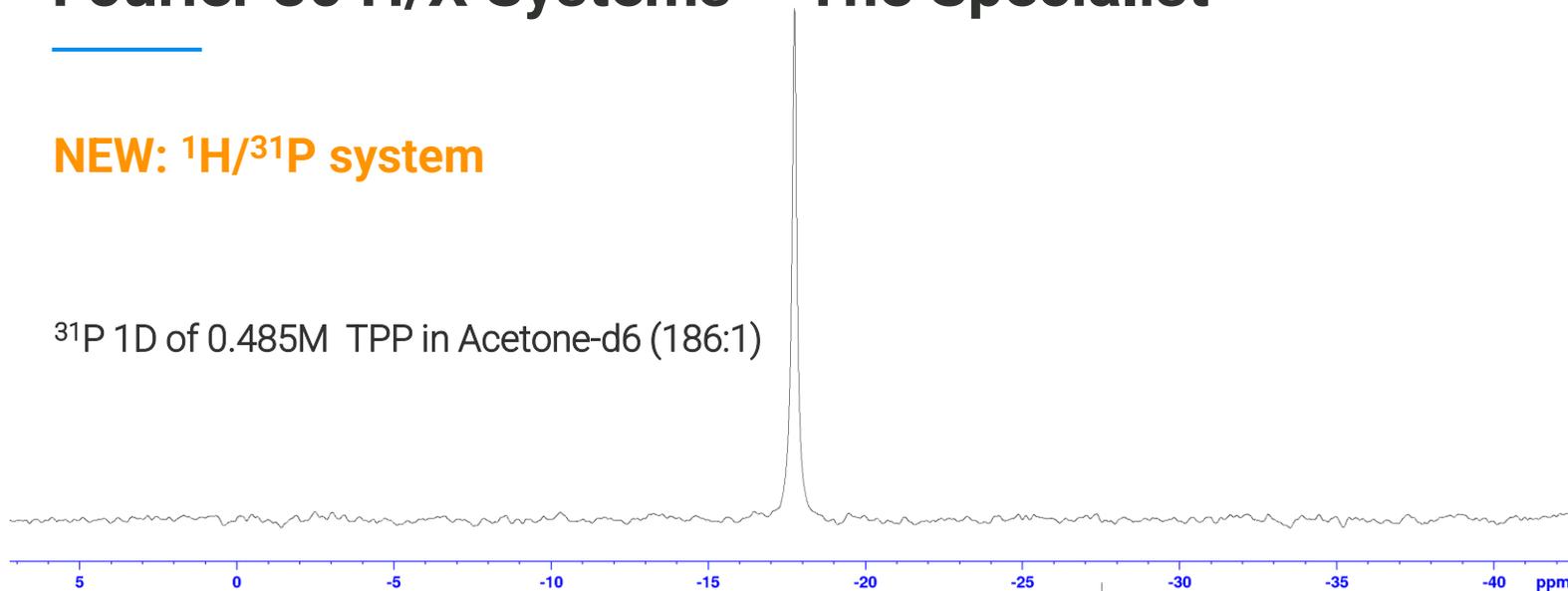
**04** The Specialist  
H/X system (X-optimized S/N)



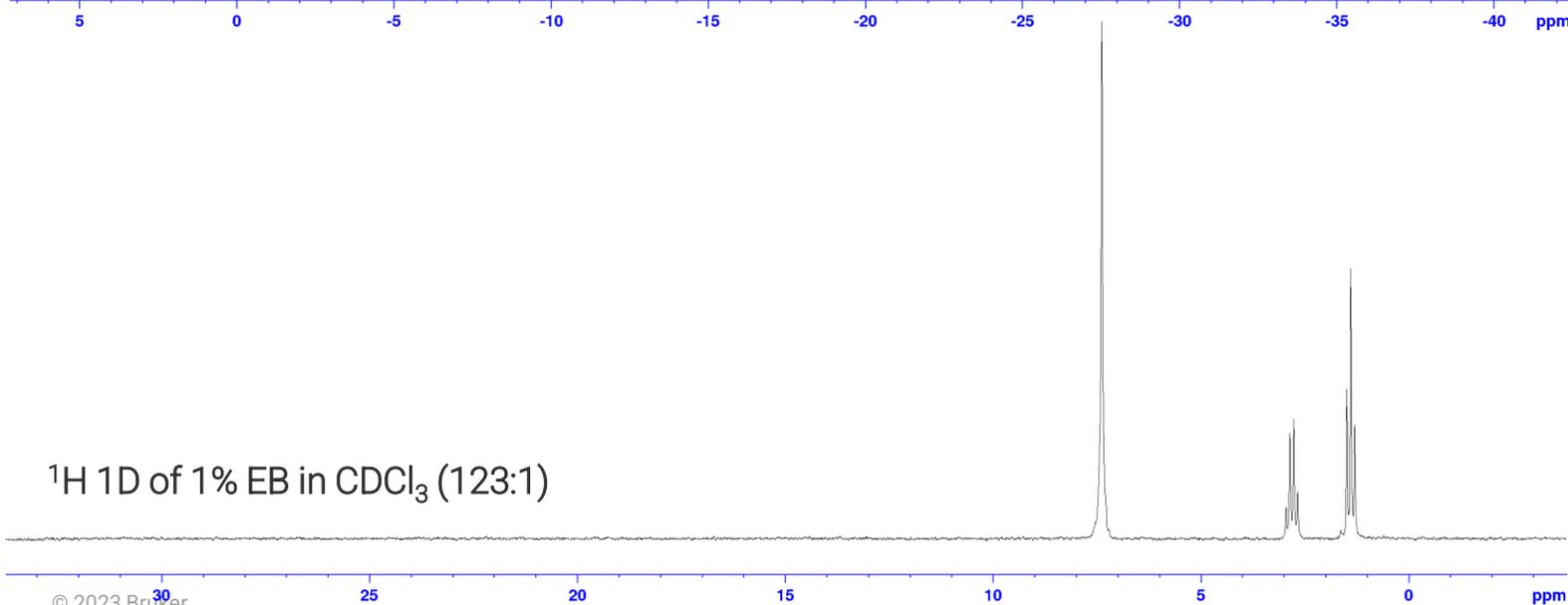
## Fourier 80 H/X Systems – The Specialist

### NEW: $^1\text{H}/^{31}\text{P}$ system

$^{31}\text{P}$  1D of 0.485M TPP in Acetone-d<sub>6</sub> (186:1)



$^1\text{H}$  1D of 1% EB in  $\text{CDCl}_3$  (123:1)

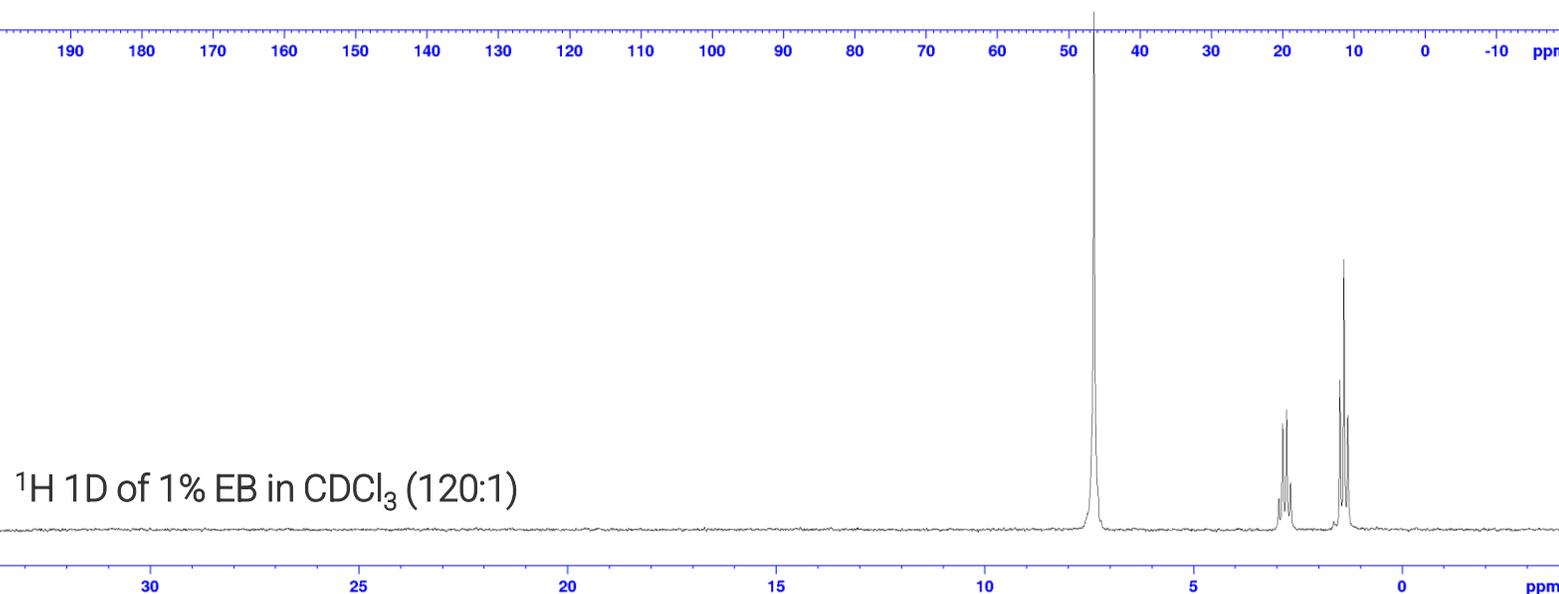
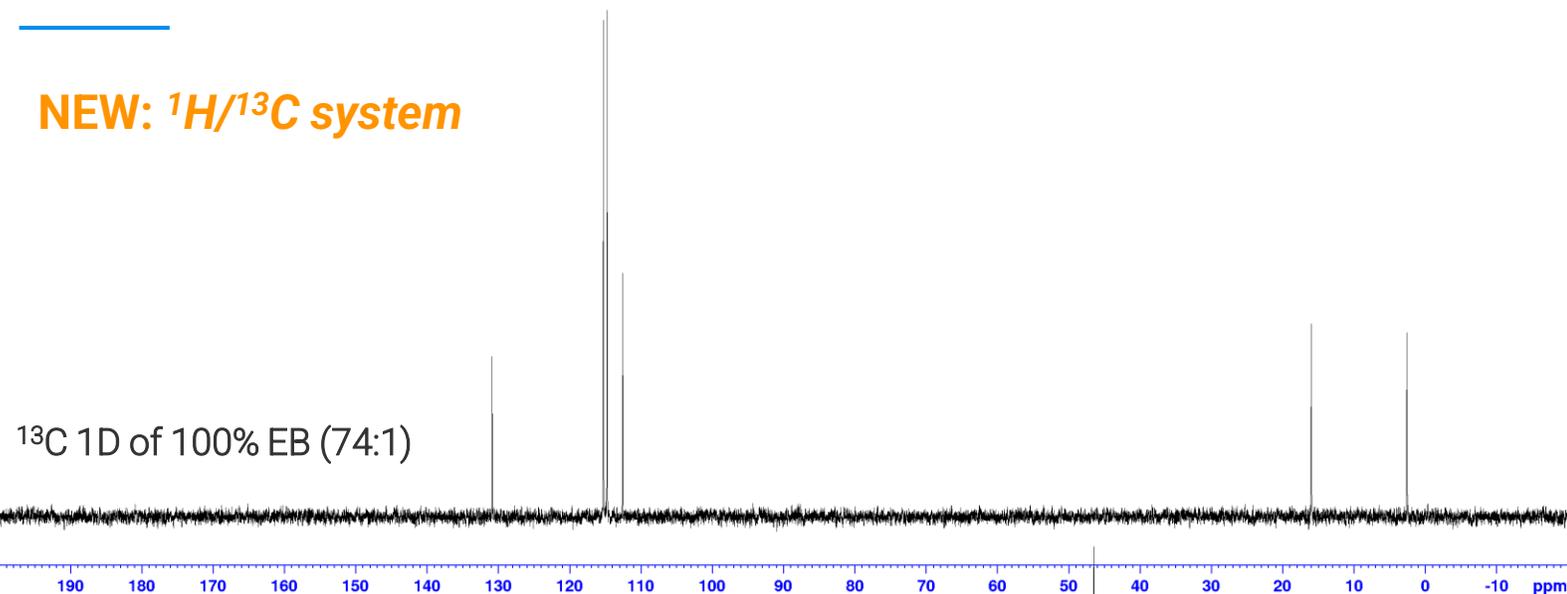


- Double channel system for direct detection of:
  - $^1\text{H}$  with X dec.
  - X with  $^1\text{H}$  dec.
- X-optimized sensitivity
- $^1\text{H}/^{31}\text{P}$  system:
  - ≥ 130:1 for  $^{31}\text{P}$
  - ≥ 90:1 for  $^1\text{H}$

Other H/X systems available:  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{29}\text{Si}$ ,  $^{11}\text{B}$

## Fourier 80 H/X Systems – The Specialist

### NEW: $^1\text{H}/^{13}\text{C}$ system



- Double channel system for direct detection of:
  - $^1\text{H}$  with X dec.
  - X with  $^1\text{H}$  dec.
- X-optimized sensitivity
- $^1\text{H}/^{13}\text{C}$  system:
  - $\geq 65:1$  for  $^{13}\text{C}$
  - $\geq 90:1$  for  $^1\text{H}$

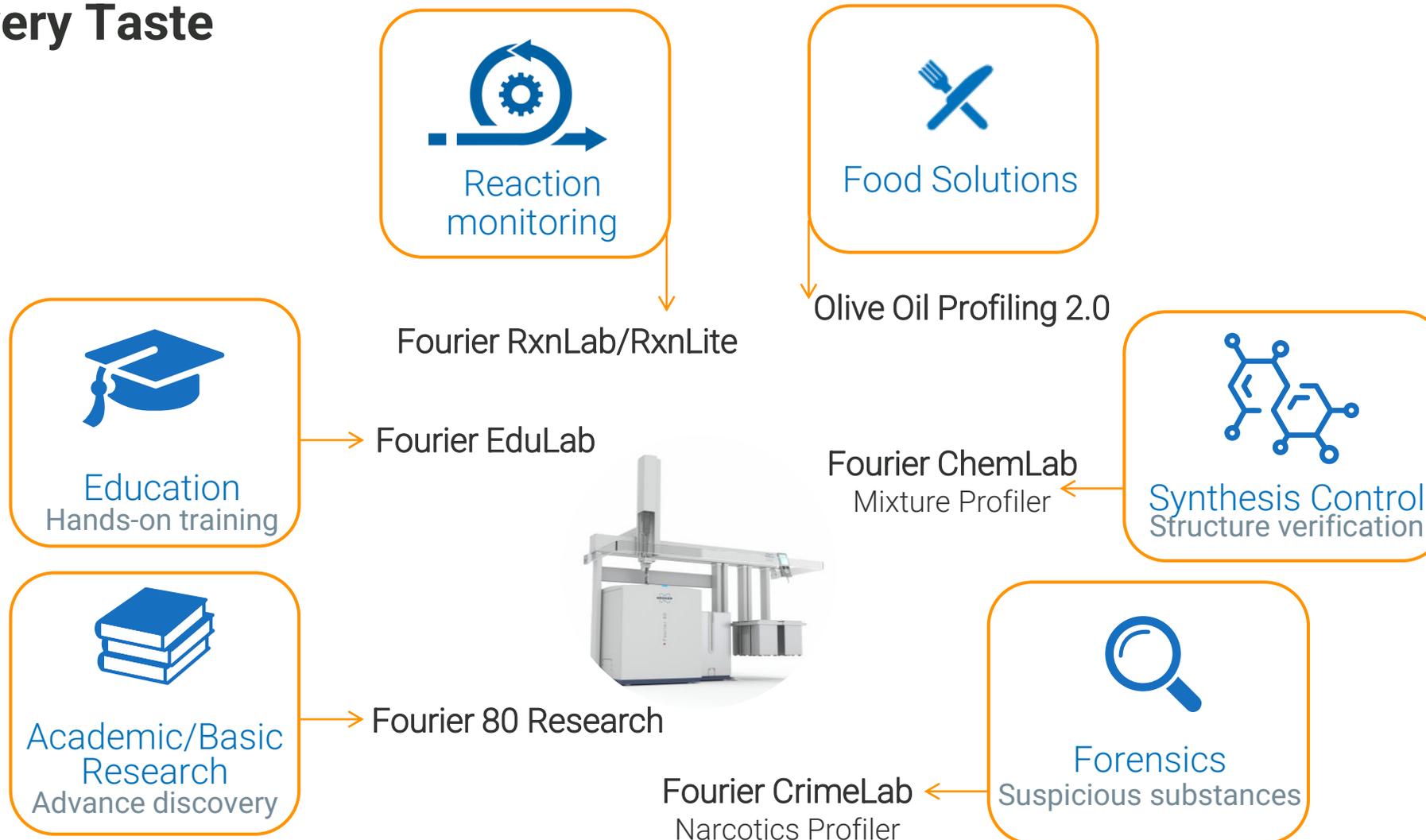
Other H/X systems available:  $^7\text{Li}$ ,  $^{23}\text{Na}$ ,  $^{29}\text{Si}$ ,  $^{11}\text{B}$

FOURIER 80 – PRODUCT UPDATES

# Fourier 80 – Flavors at a Glance

---

# Flavors for Every Taste



FOURIER 80 – PRODUCT UPDATES

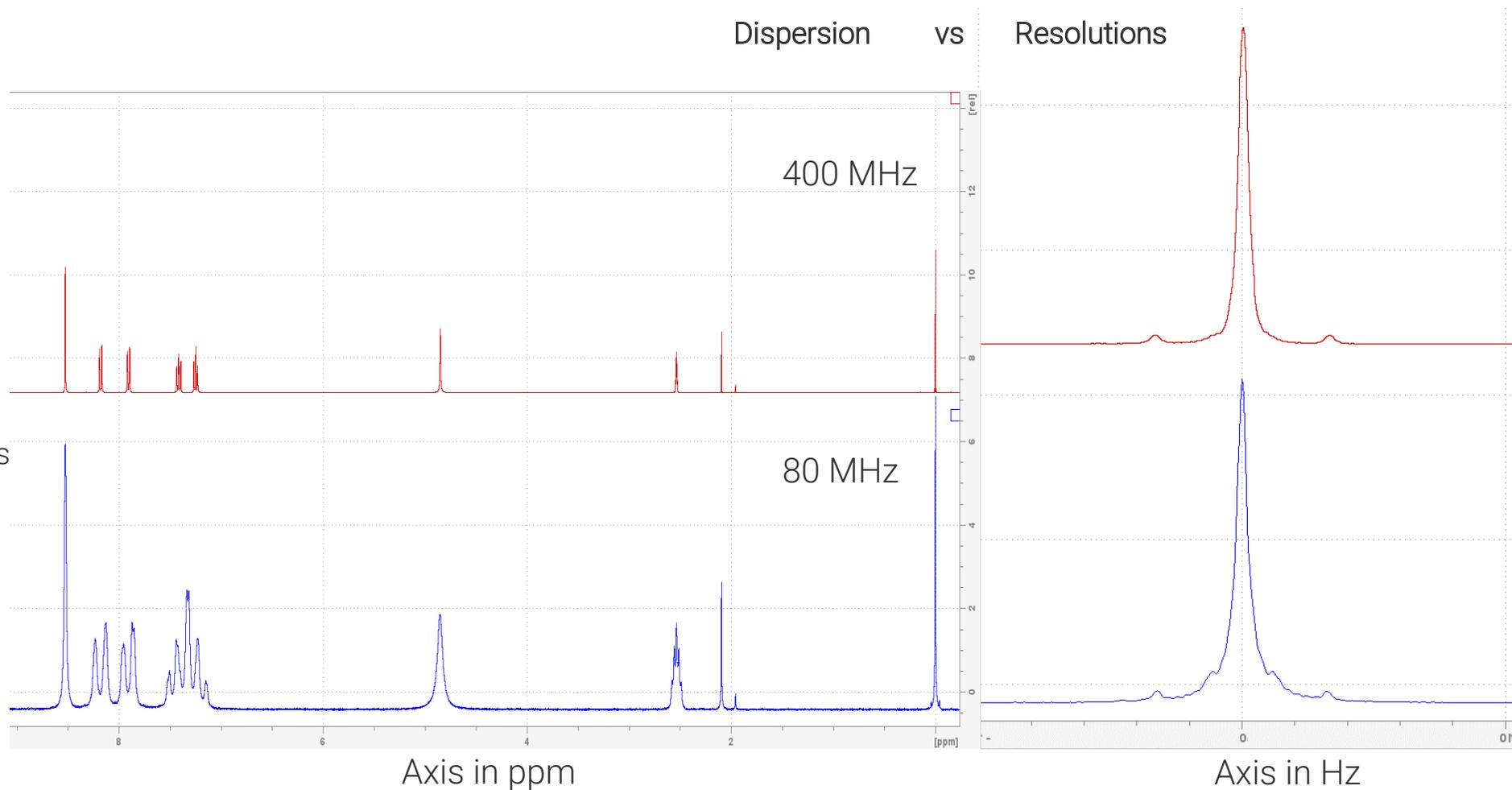
# Fourier 80 – Tips and Tricks

---

# 80 MHz – What to Expect



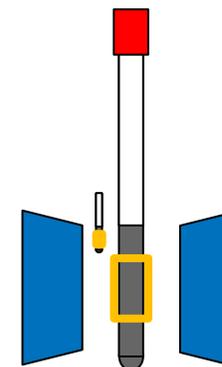
Sensitivity ( $^1\text{H}$  SNR):  
400 MHz vs 80 MHz ~ 30x less



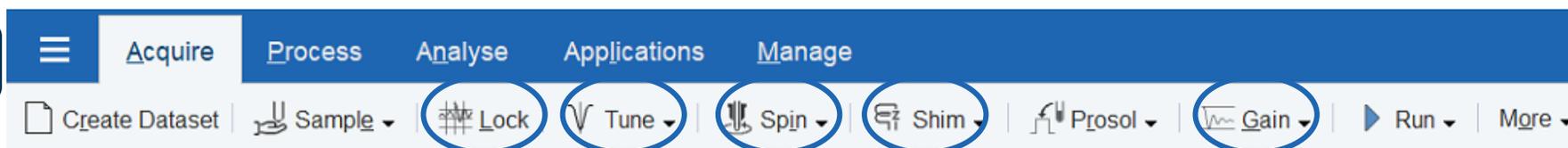
# Practical Aspects

## External lock

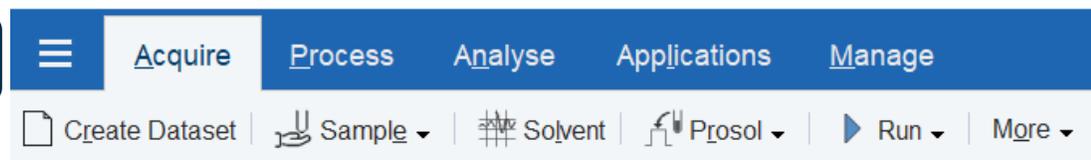
- No deuterated solvents needed
- NMR-signal of substance in lock capillary is measured constantly
- Sample and lock sample are spatially separated
- Lock experiences slightly different effects



400 MHz



80 MHz



- no tuning and matching: tune/match are factory settings
- no shimming on each sample
- no gain – set automatically

# Practical Aspects – Solvent Suppression

## Opportunities

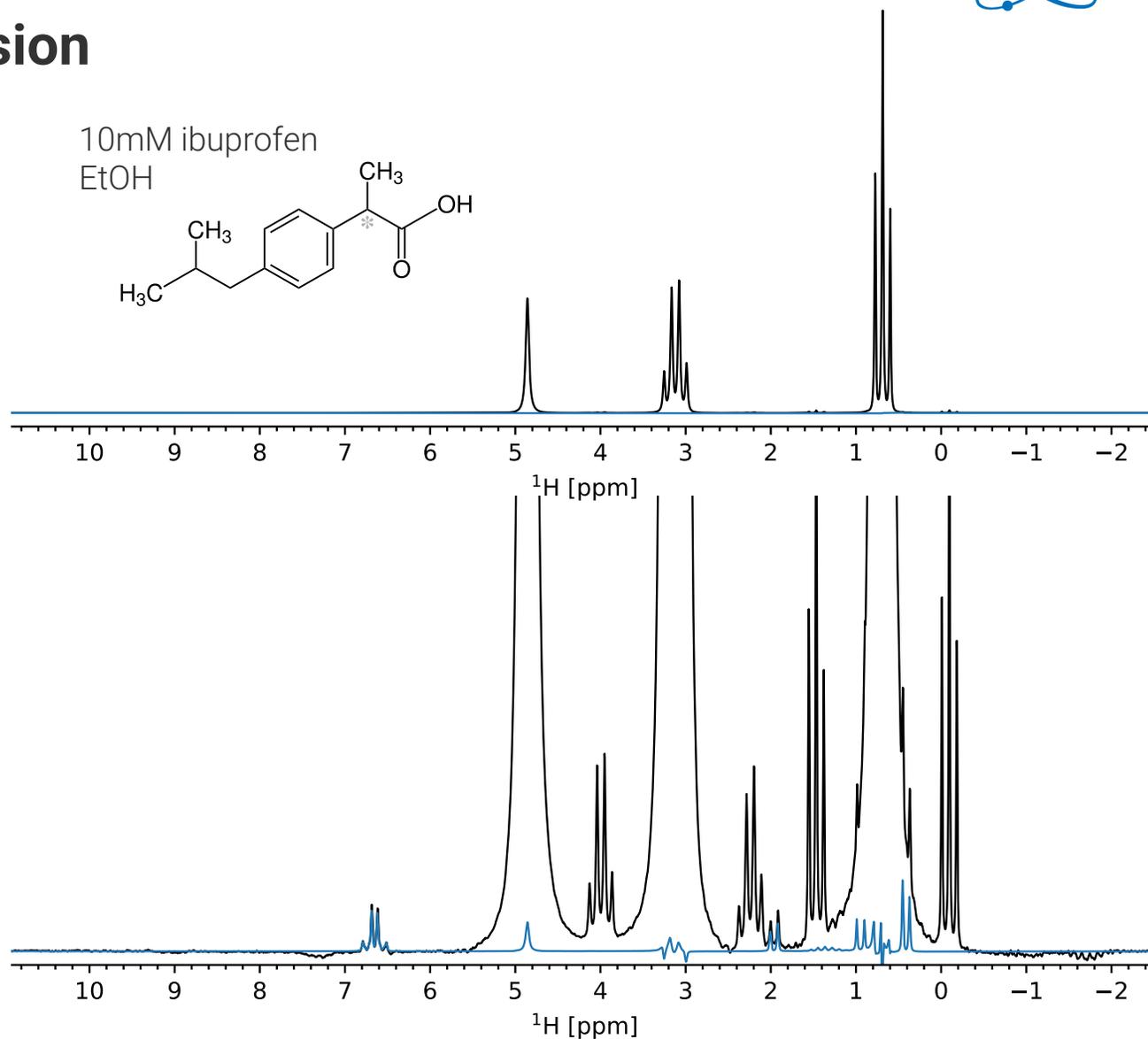
- External lock -> no need for D
- Measure liquid samples with no alteration
- Save time & deuterated solvents

## Challenges

- Solvents with multiple strong signals
- Large multiplets due to low field
- $^{13}\text{C}$  satellites at almost  $\pm 1$  ppm

## Result

- Runs in full automation
- Compatible with GoScan
- Applicable at all fields



FOURIER 80 – PRODUCT UPDATES

# Fourier 80 – Application Examples

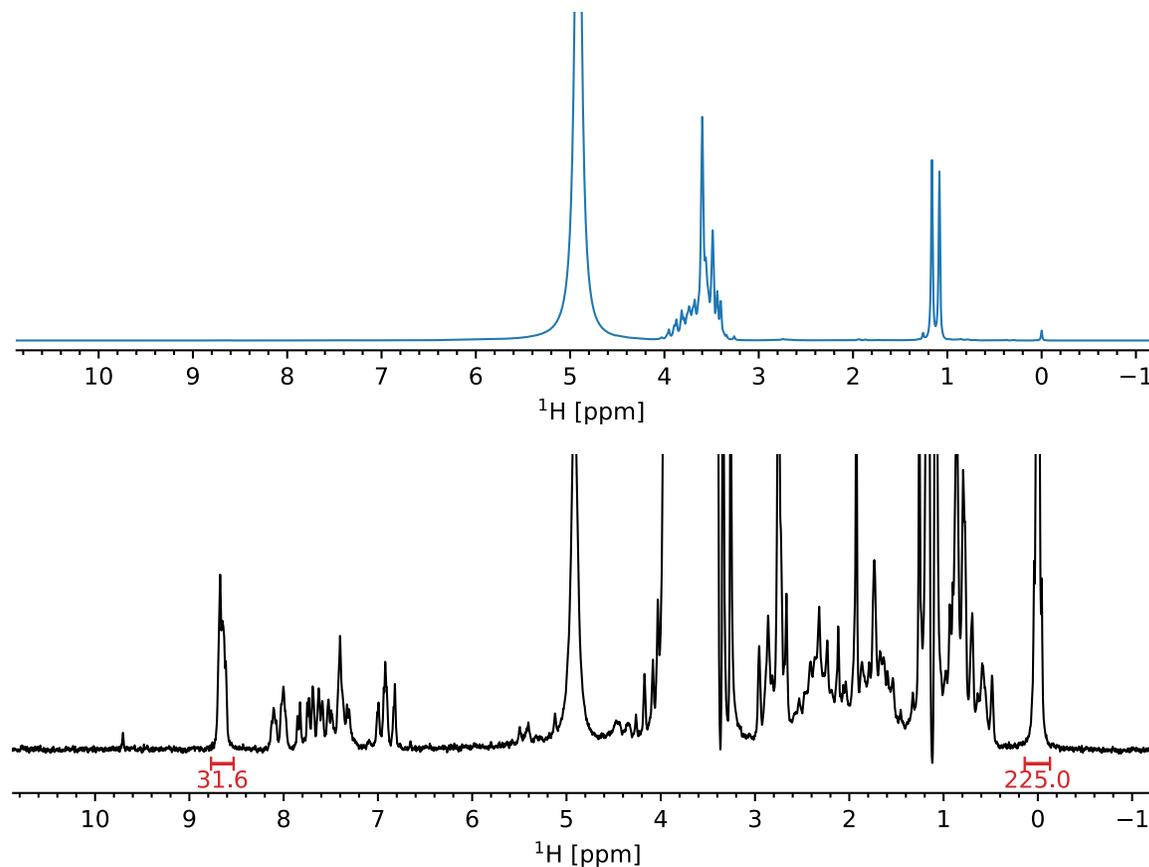
---

# Application Examples



## Nicotine Quantification of e-Cigarette liquids:

- Nicotine in H<sub>2</sub>O/Glycerol/Propyleneglycol
- Mix 1:1 with 50 mM DSS in H<sub>2</sub>O
- Acquire spectrum with multiple suppression
- Quantify DSS vs nicotine

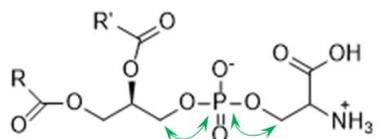


# Application Examples



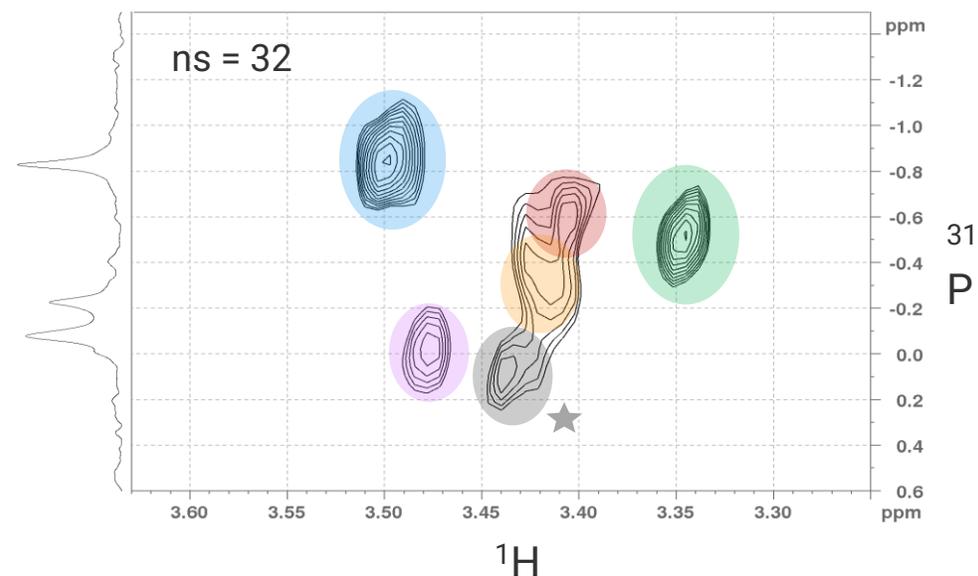
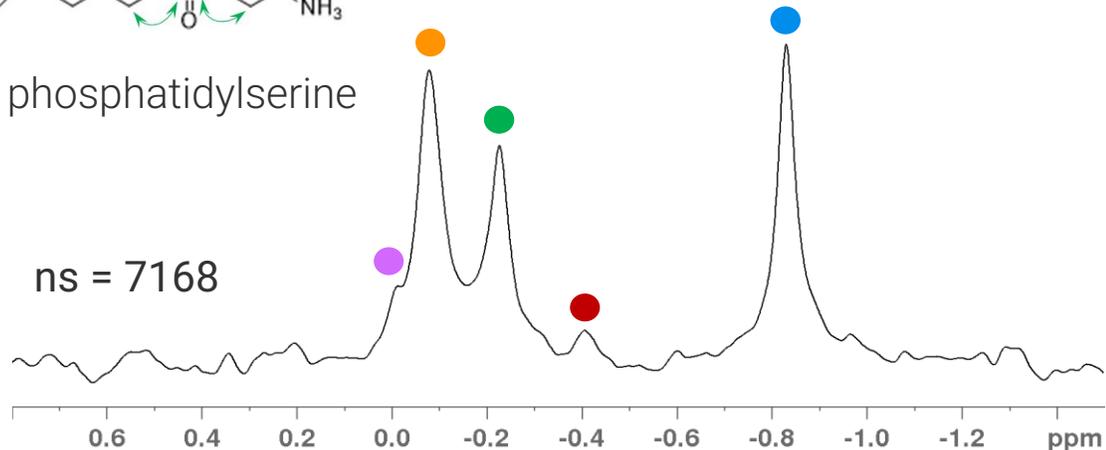
## Detecting phospholipids in whey extracts using $^{31}\text{P}$ -NMR:

- sphingomyeline \*
- phosphatidylethanolamine (cephalin) \*
- phosphatidylserine \*
- phosphatidylinositol \*
- phosphatidylcholine (lecithin)



phosphatidylserine

ns = 7168



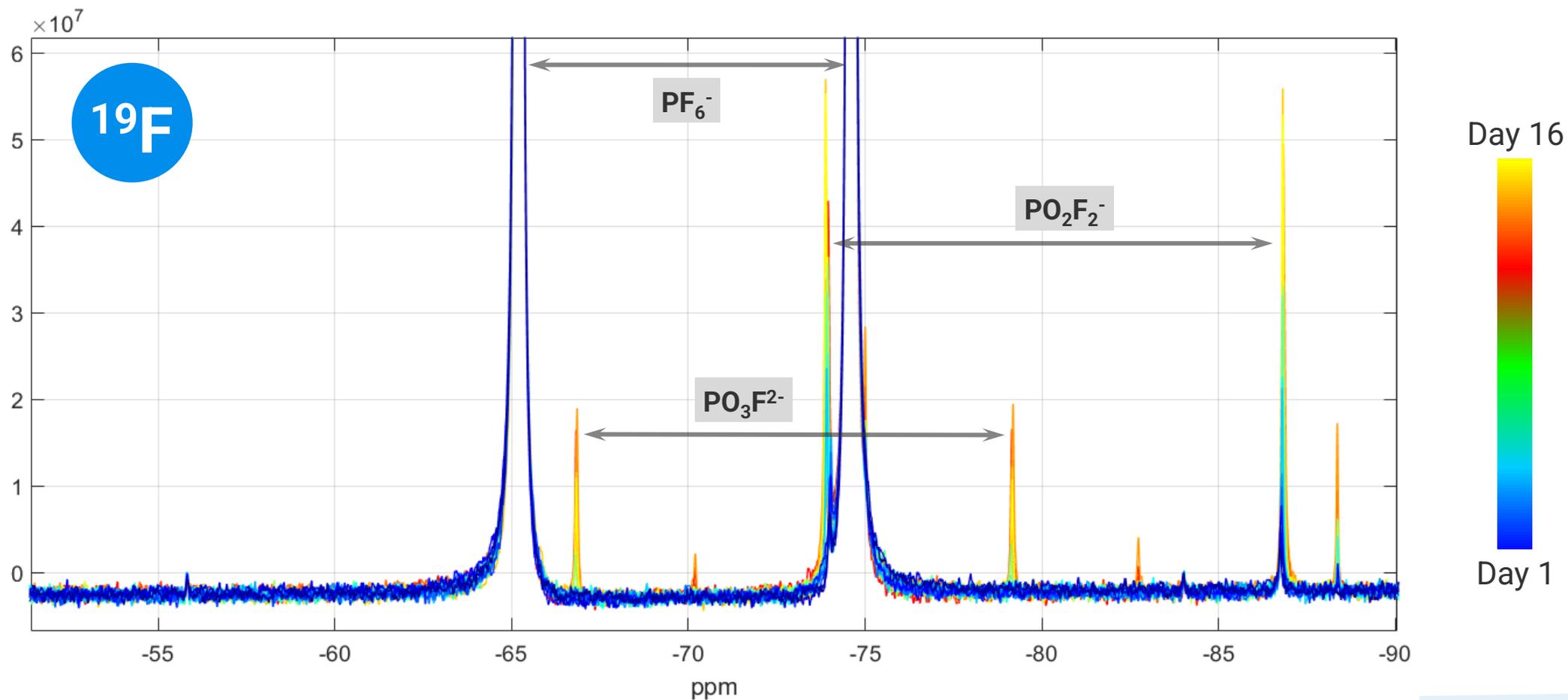
- applying the  $^1\text{H}$ - $^{31}\text{P}$  HMBC (shows correlation peaks between the P and H atoms, as marked in the molecular structure) reduces the experimental time significantly
- a sixth phospholipid signal, which still is hidden in the  $^{31}\text{P}$  spectrum, appears in the HMBC

# Application Examples



$^{19}\text{F}$

Tracking electrolyte degradation:



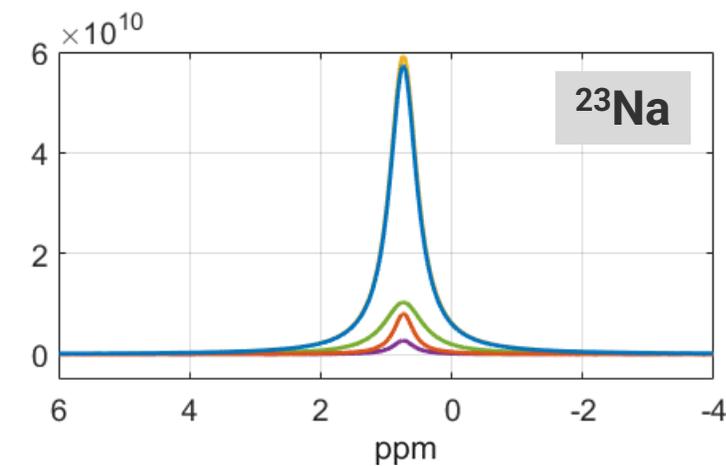
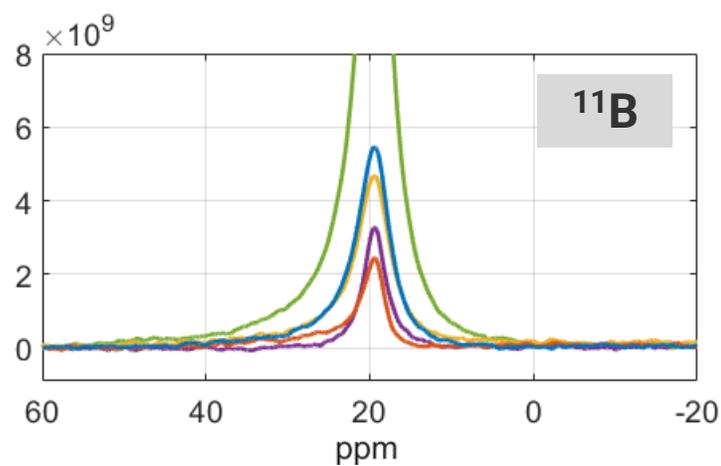
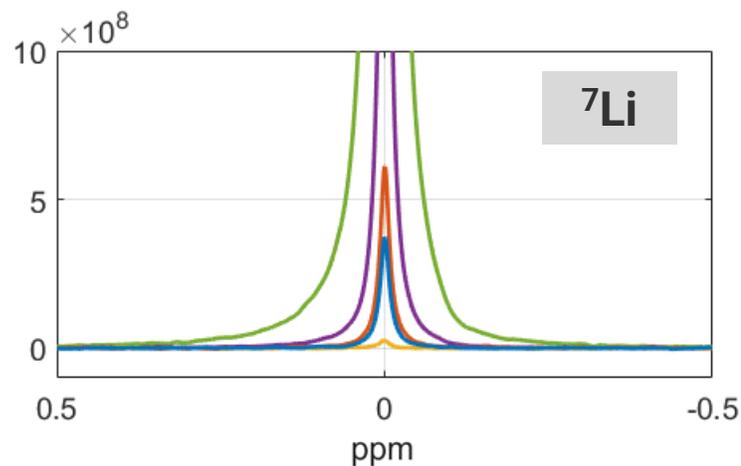
# Application Examples



## Quantification of cations in brines:

- Lithium extraction
- for economic mining of lithium, the brines' lithium contents must be known (higher = better)
- but brines contain further cations, which are undesired - like sodium and boron; their content also must be known

Quantification of  $^7\text{Li}$ ,  $^{11}\text{B}$  and  $^{23}\text{Na}$  in natural and processed brines with the Fourier 80 Benchtop



# Conclusions

## Small but Mighty



EDULAB FOR STUDENTS: FOURIER 80  
**The Caffeine Kick**  
NMR of Coffee



EDULAB FOR STUDENTS: FOURIER 80  
**Milky way to NMR**  
NMR Analysis of Milk

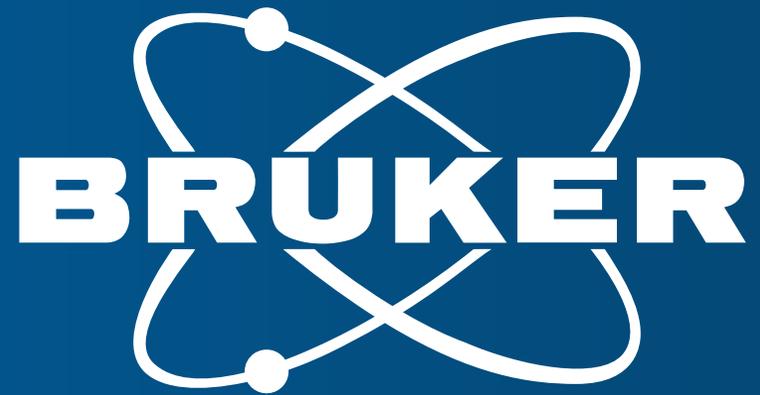




# Thank you!

---

Tangi.jezequel@bruker.com

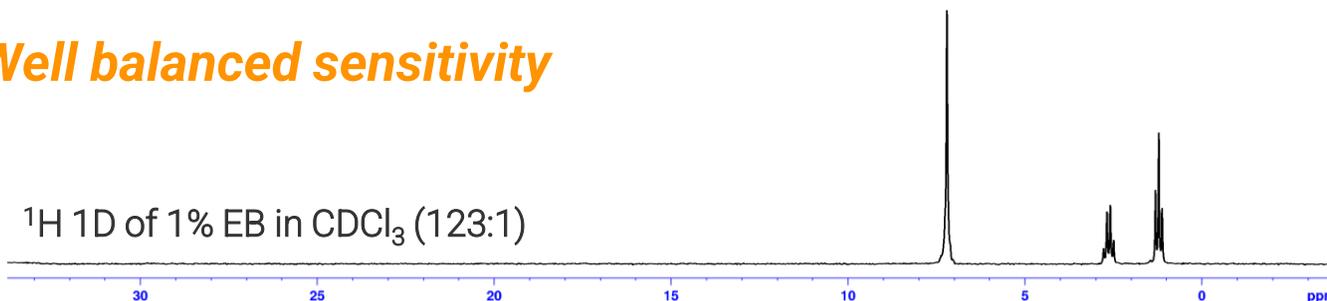


Innovation with Integrity

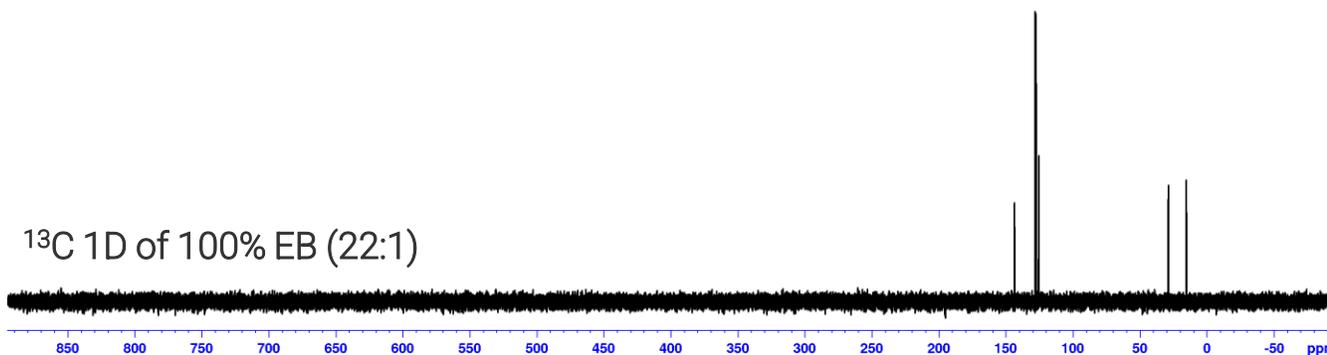
## Fourier 80 H/C|F system – The multi-talent

### Well balanced sensitivity

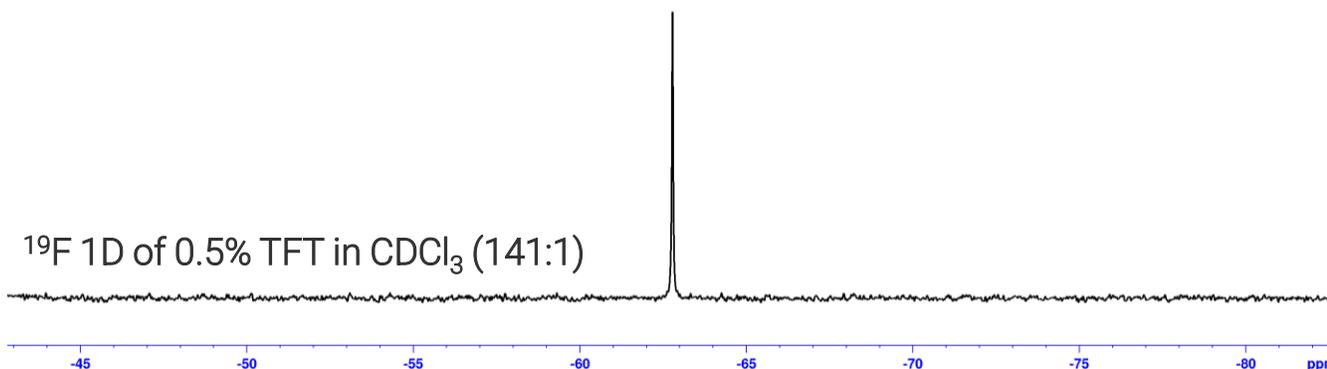
$^1\text{H}$  1D of 1% EB in  $\text{CDCl}_3$  (123:1)



$^{13}\text{C}$  1D of 100% EB (22:1)



$^{19}\text{F}$  1D of 0.5% TFT in  $\text{CDCl}_3$  (141:1)



- Double channel system with double-tuned X channel for direct detection of:
  - $^1\text{H}$  with  $^{13}\text{C}$  or  $^{19}\text{F}$  dec.
  - $^{19}\text{F}$  with  $^1\text{H}$  dec.
  - $^{13}\text{C}$  with  $^1\text{H}$  dec.
- Well-balanced sensitivity:
  - $\geq 110:1$  for  $^{19}\text{F}$
  - $\geq 20:1$  for  $^{13}\text{C}$
  - $\geq 110:1$  for  $^1\text{H}$