

Thermophoresis of cyclodextrins with/without aspirin in water

K. Eguchi¹, D. Niether², J. Hovancova³, T. Kawaguchi¹, R. Kita¹ and S. Wiegand^{2,4}

¹School of Science, Tokai University, Hiratsuka Kanagawa 259-1292, Japan

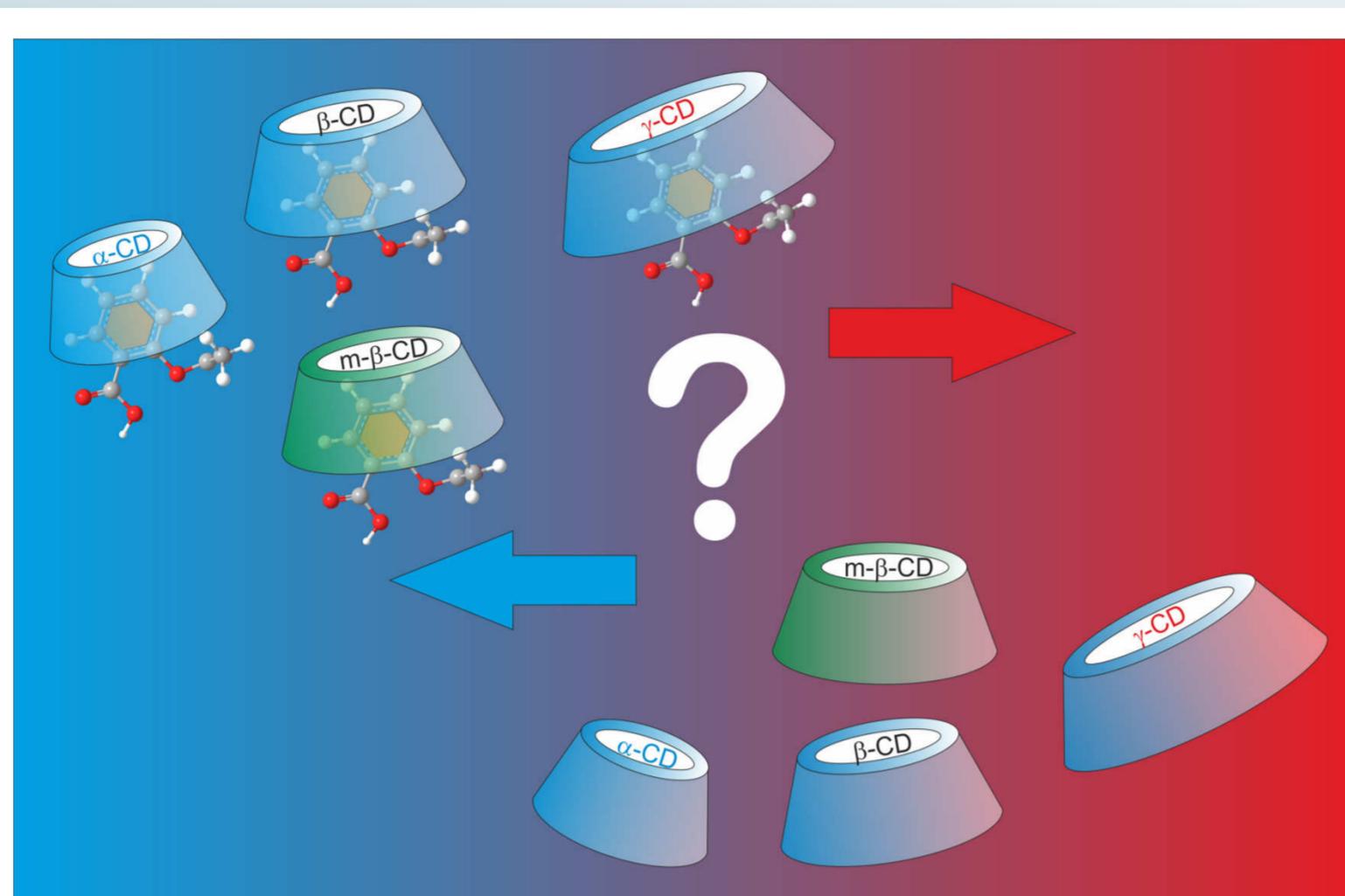
²ICS-3 Soft Condensed Matter, Forschungszentrum Jülich GmbH, D-52428 Jülich, Germany

³Chemistry Department, Pavol Jozef Šafárik University, Košice, Slovakia

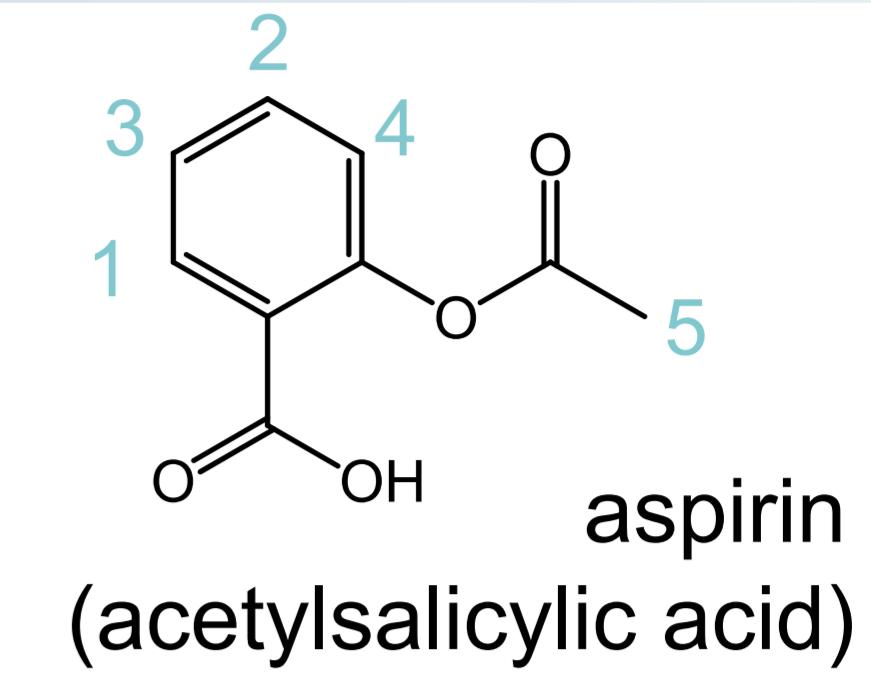
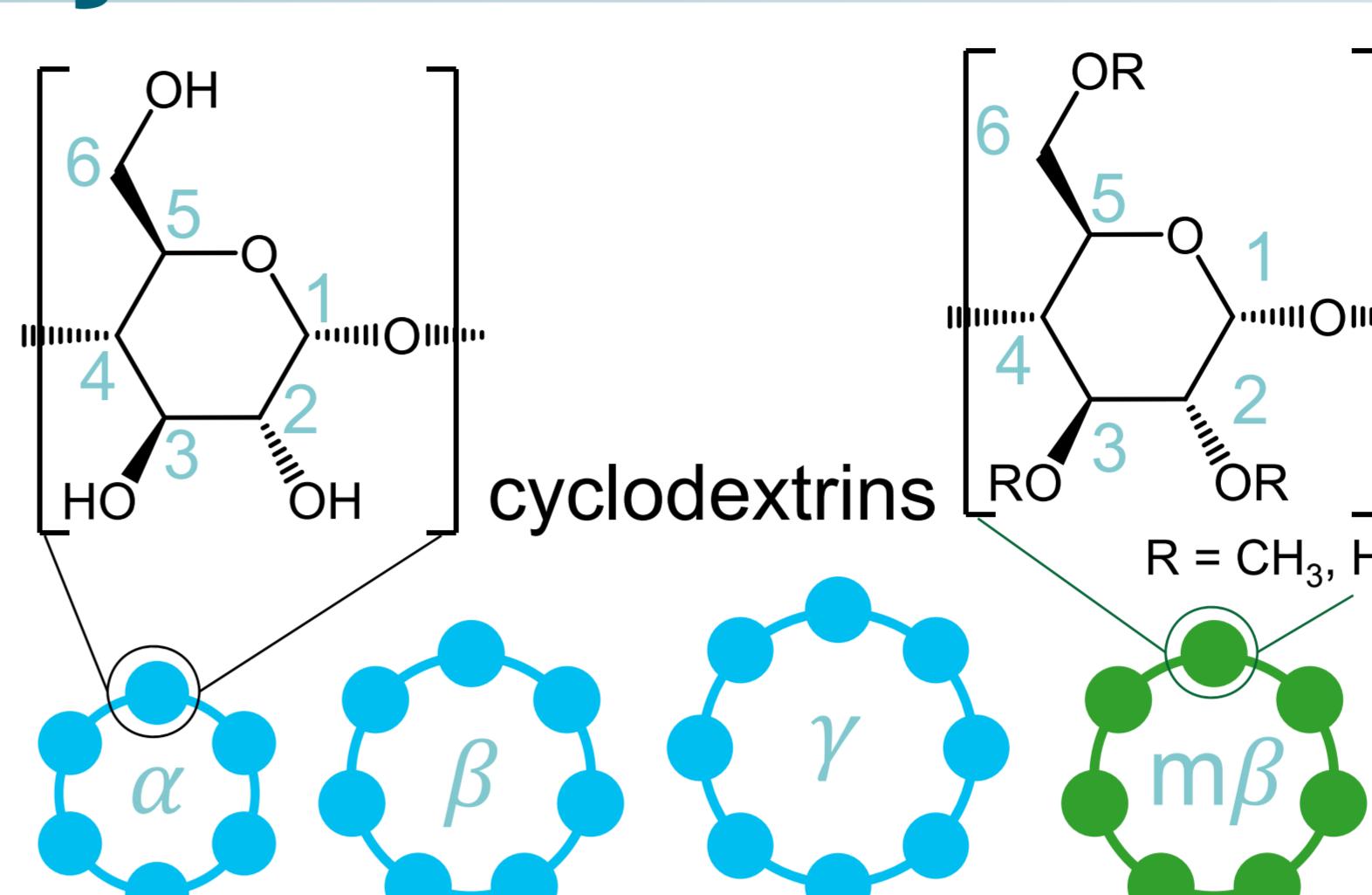
⁴Chemistry Department – Physical Chemistry, University Cologne, D-50939 Cologne, Germany

Motivation [1]

- Controlled movement of drugs into certain, e.g. inflamed, areas
- Check complex formation: α -, β -, γ - and methyl- β -cyclodextrin with aspirin by NMR
- Investigation of thermophoretic behavior

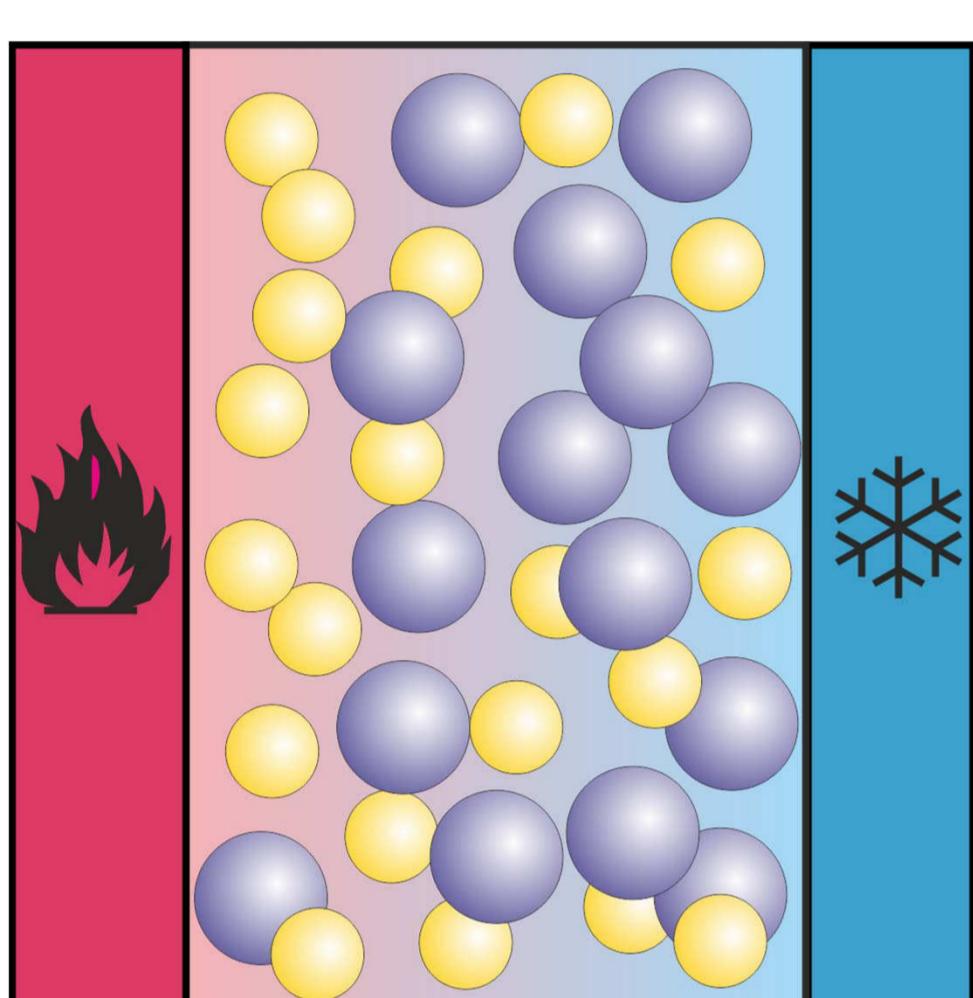


System



concentration: 1wt% CD
molar 1:1-ratio: CD:aspirin

Thermophoresis [2]



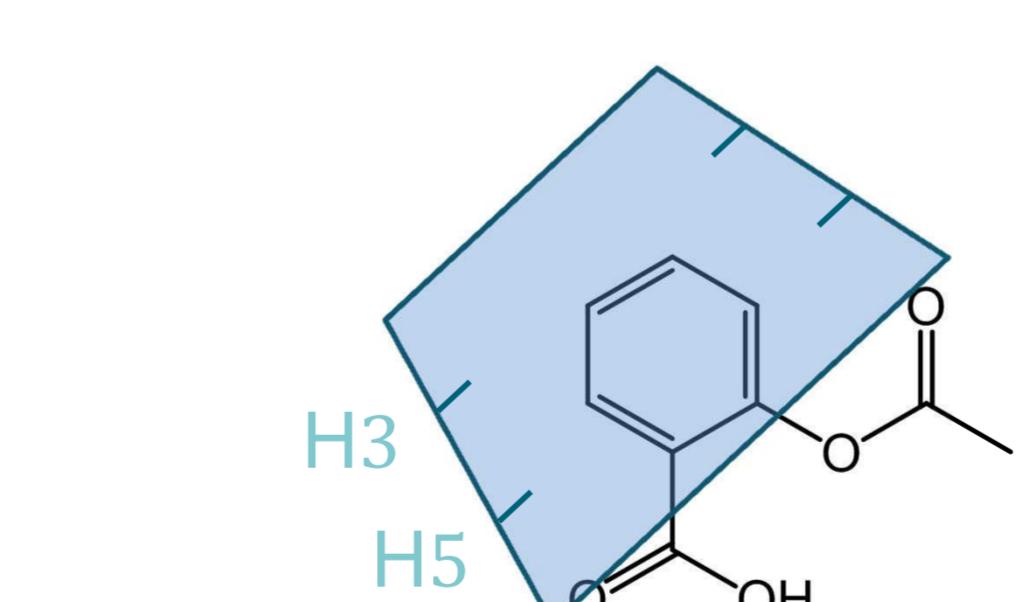
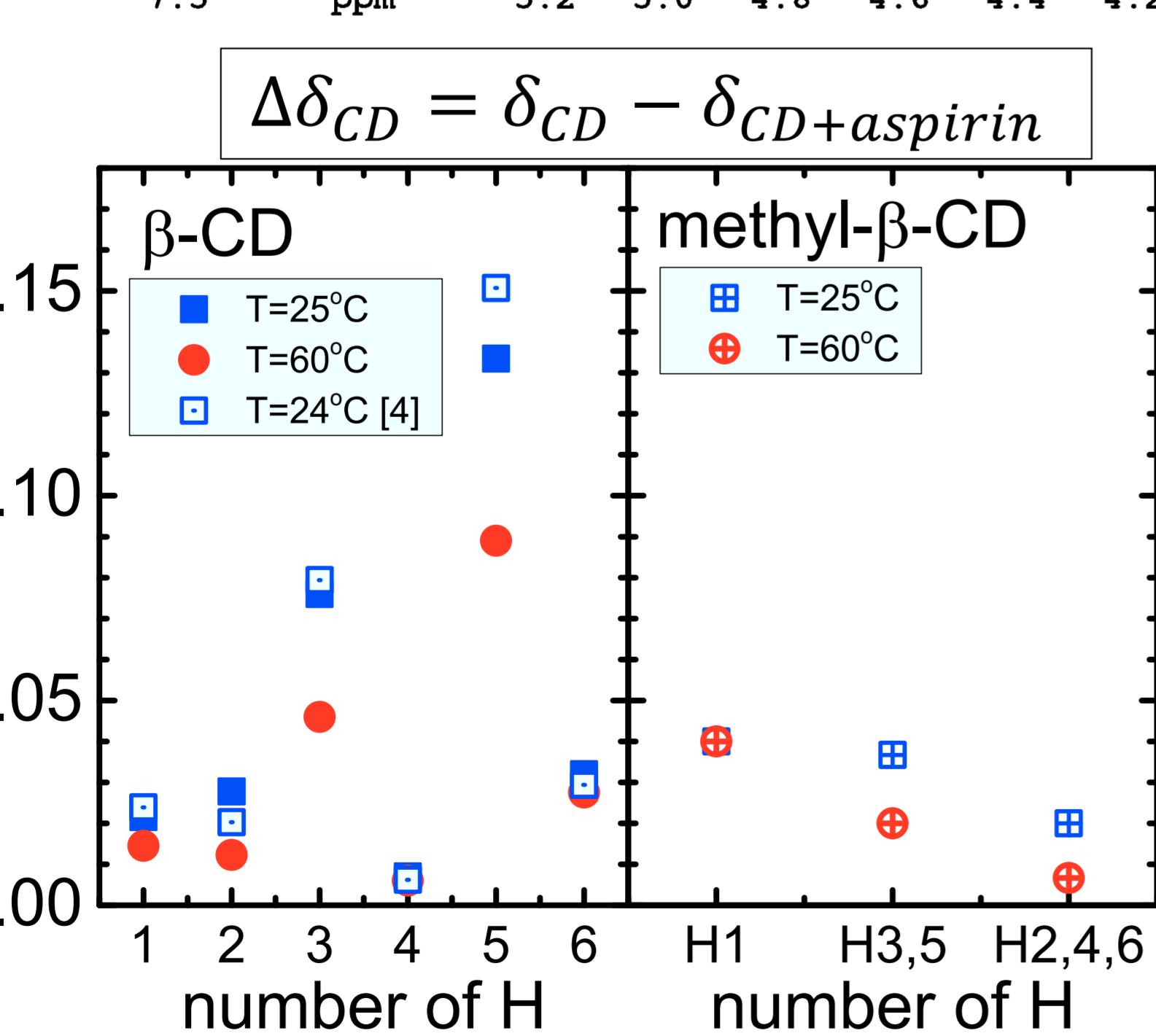
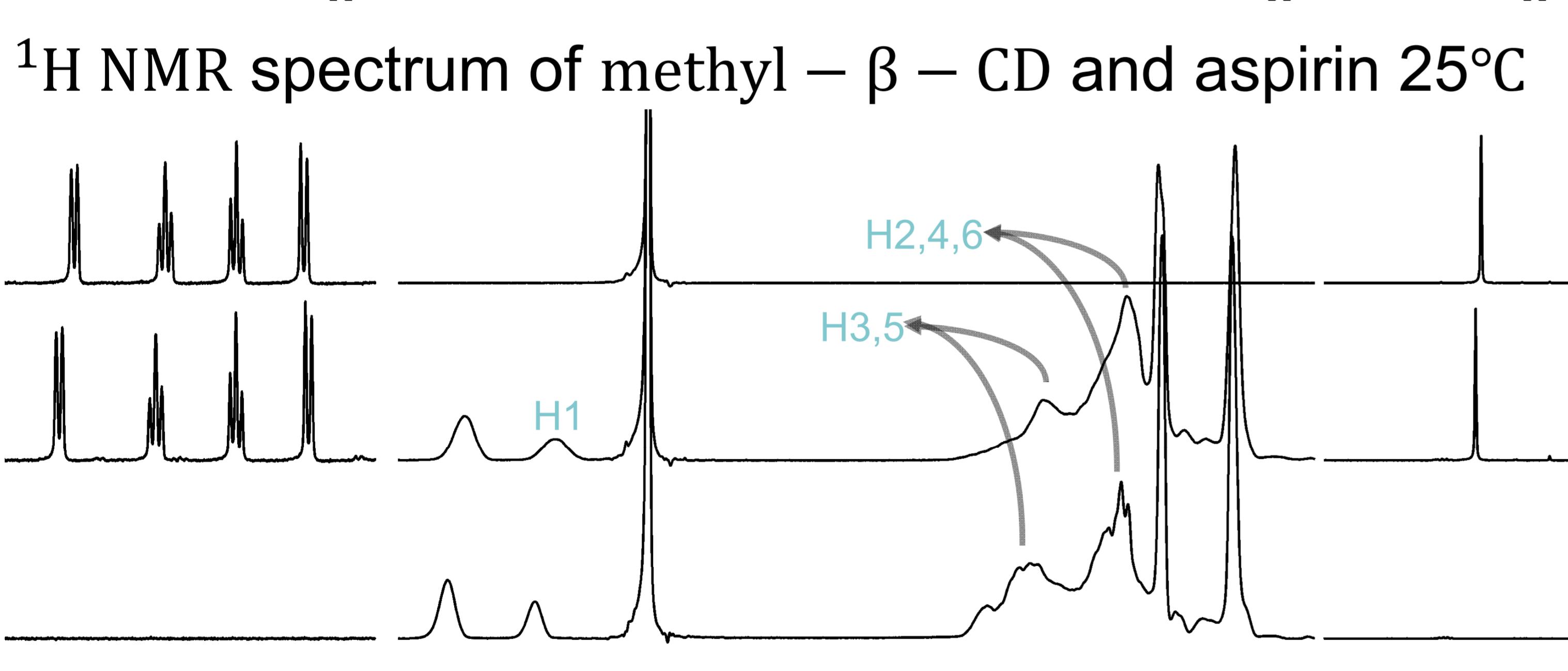
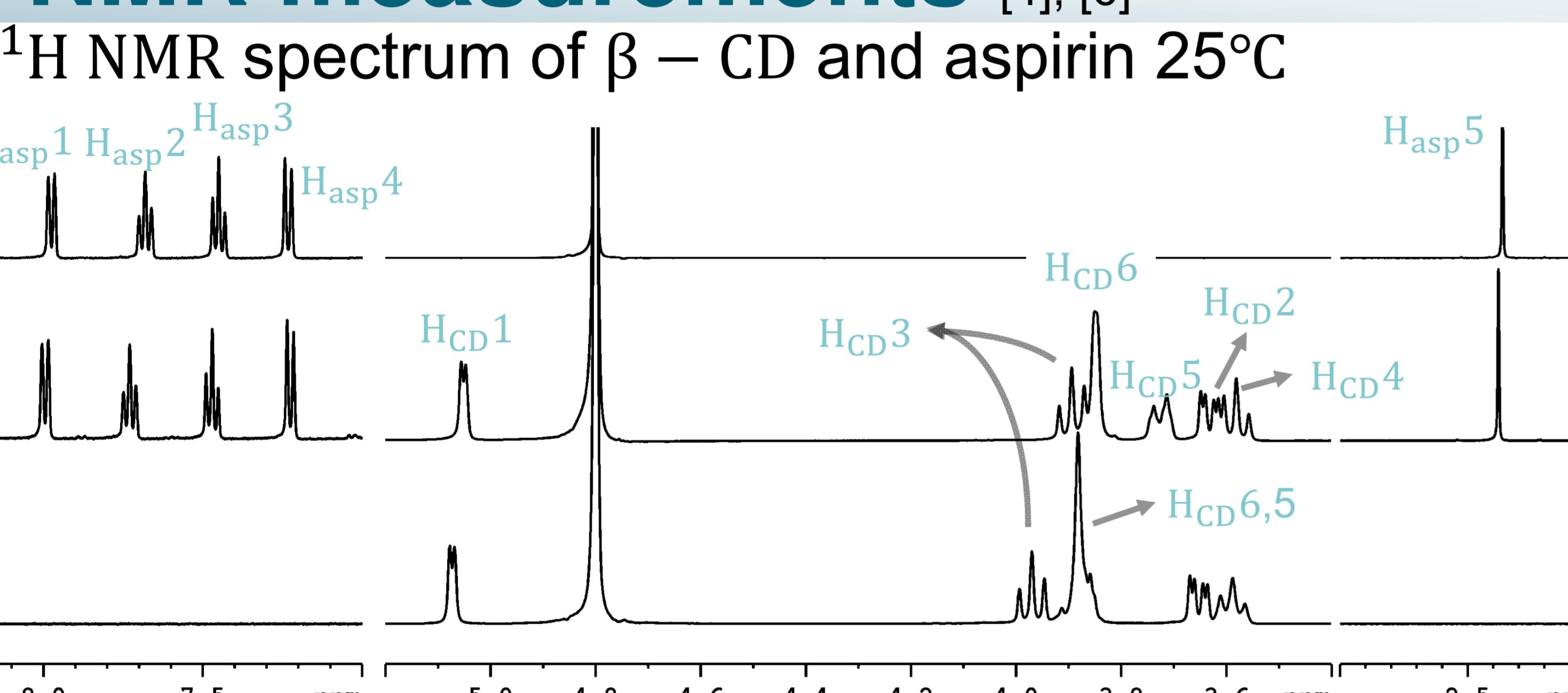
Flux j along a temperature gradient:
 (1) thermal diffusion D_T along a temperature gradient ∇T
 (2) Fickian diffusion D along the induced concentration gradient ∇c .

$$\vec{j} = -D\vec{\nabla}c - c(1-c)D_T\vec{\nabla}T$$

In the steady state ($j=0$) the Soret coefficient S_T is defined

$$S_T \equiv \frac{D_T}{D} = -\frac{1}{c(1-c)} \frac{\Delta c}{\Delta T}$$

NMR measurements [4], [6]



Magnetic field of inwards pointing protons (H3 and H5) is influenced by aspirin(guest molecule).

β -CD

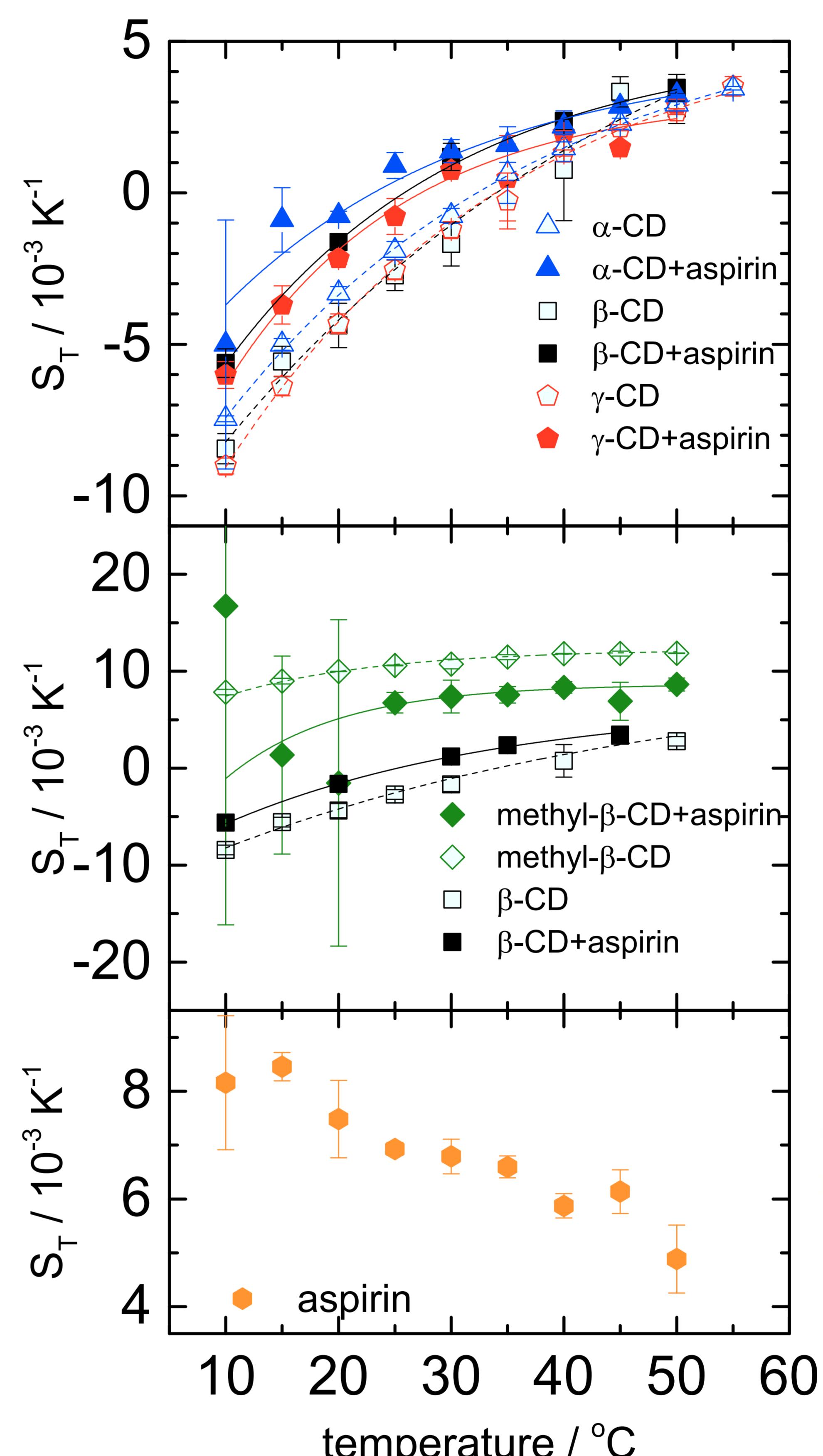
- large $\Delta\delta$ value is observed for H3 and H5 compared to the other protons.
- $\Delta\delta$ value of H3 and H5 is decreased by heating.

methyl- β -CD

- small $\Delta\delta$ value observed for H3,5 compared to β -CDs H3 and H5.
- $\Delta\delta$ value of H3,5 is decreased by heating.

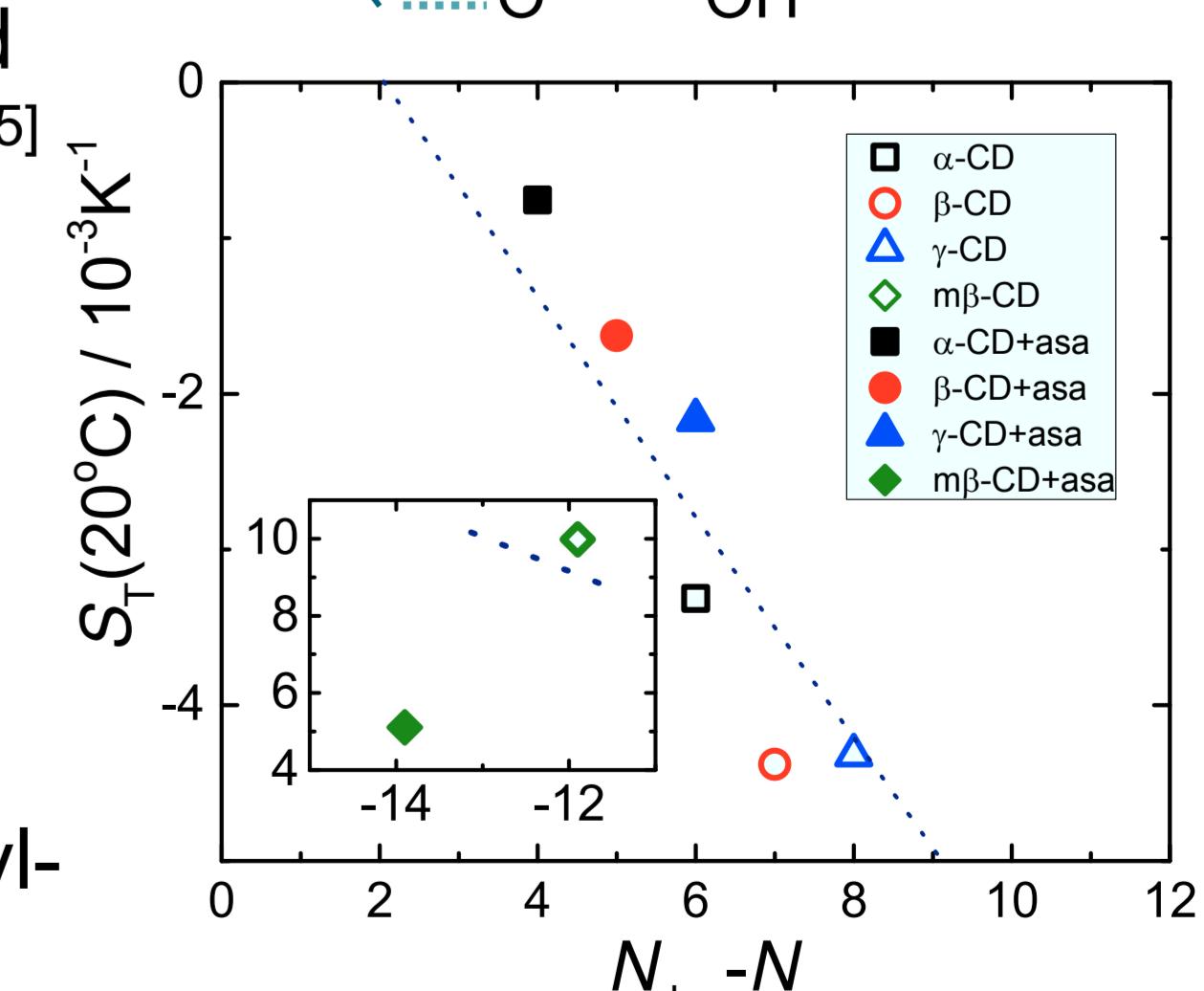
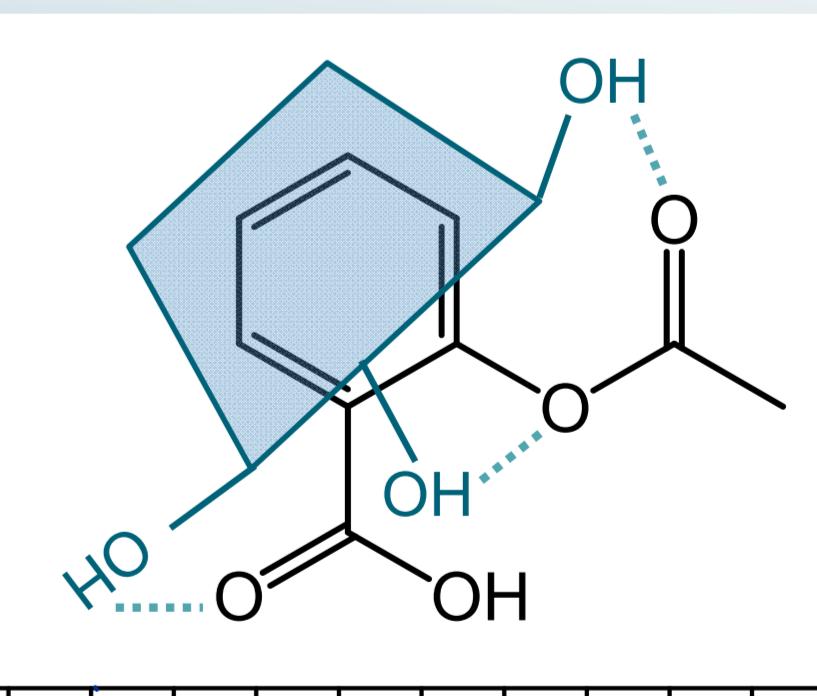
Inclusion complex is confirmed for both CDs.

TDFRS results [3]



Conclusion

- complexes formation are confirmed between CD and aspirin from NMR measurement
- At the high temperature the complex capability weakens
- behaviour of pure CDs and un-methylated CD-complexes fits donor-acceptor model^[5]
- fewer HB sites result in a higher S_T /stronger thermophobicity
- drug-complex of methyl- β -CD behaves different
- possible explanations are polarisation or charge effects
- more information about structure of methyl- β -CD-complex is needed



References

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