

# Quantitative NMR Foundation Meeting

Spectral Service



## Round Robin Tests

Do you know the performance  
of your qNMR method?

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Spectral Service AG, 10 June 2016  
Dr. Tanja Beyer

# Background

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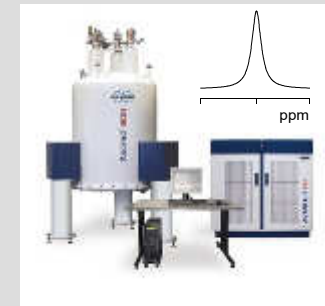


Frequently asked question in our last audits:

**“What are you doing to ensure the quality of your qNMR method as well as the technical expertise of your staff in sample preparation and evaluating quantitative NMR measurements?”**

Establishment of annual training with monitoring of success focussed on

- sample preparation
- evaluation of qNMR experiments

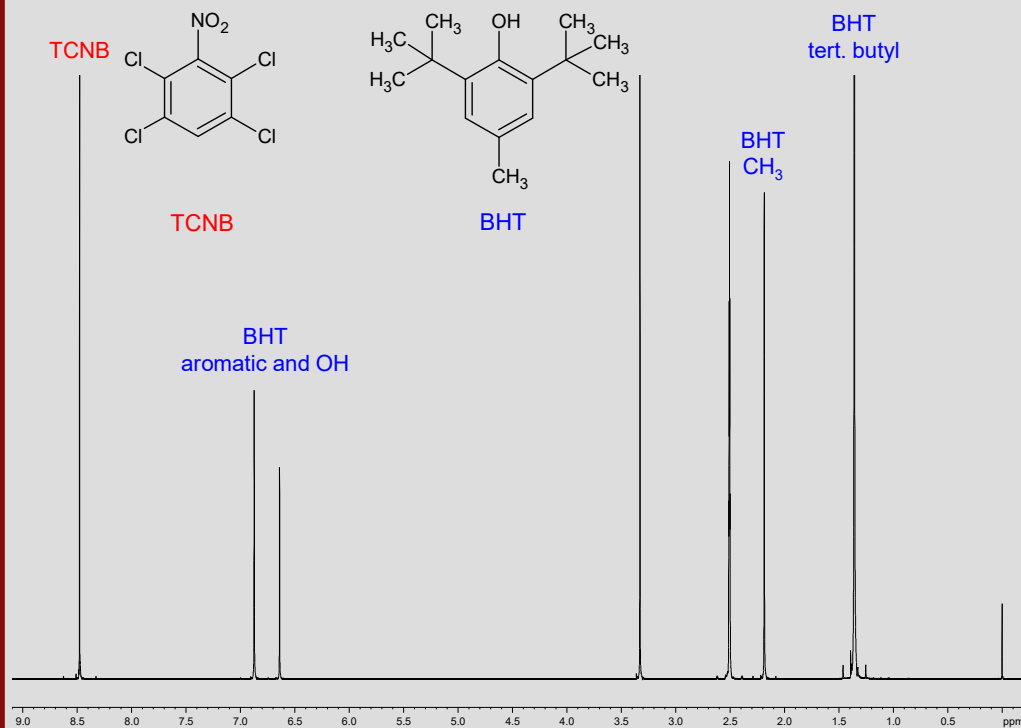
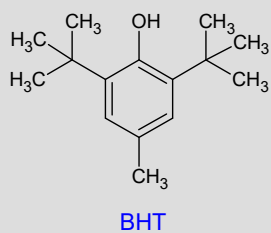
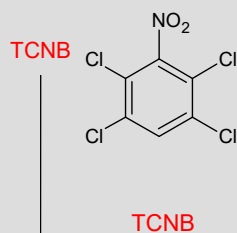


# Intralaboratory Test

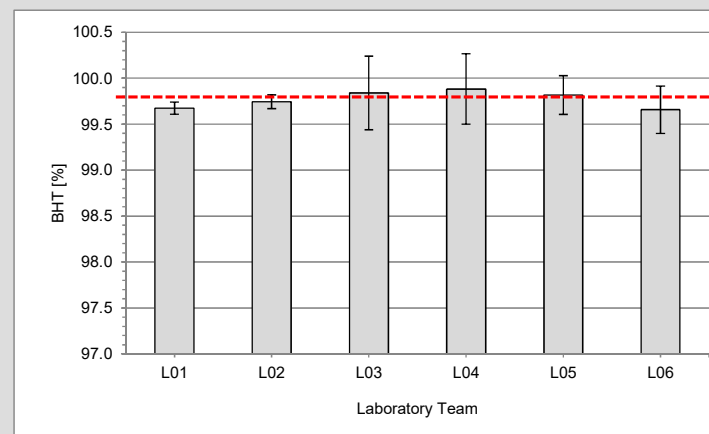
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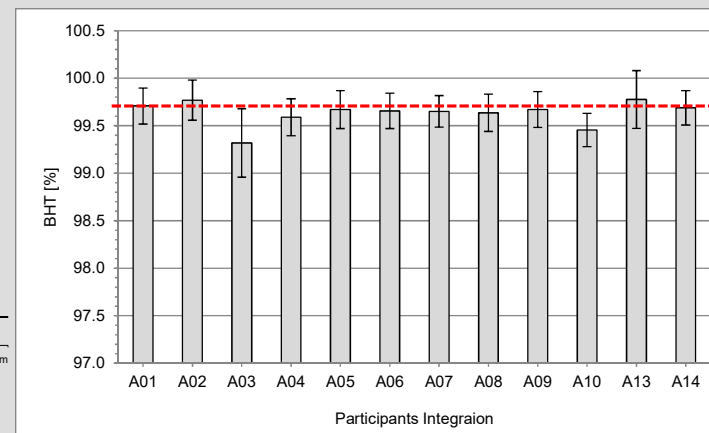
## Case study: BHT-TCNB



## Sample preparation:



## Integration:

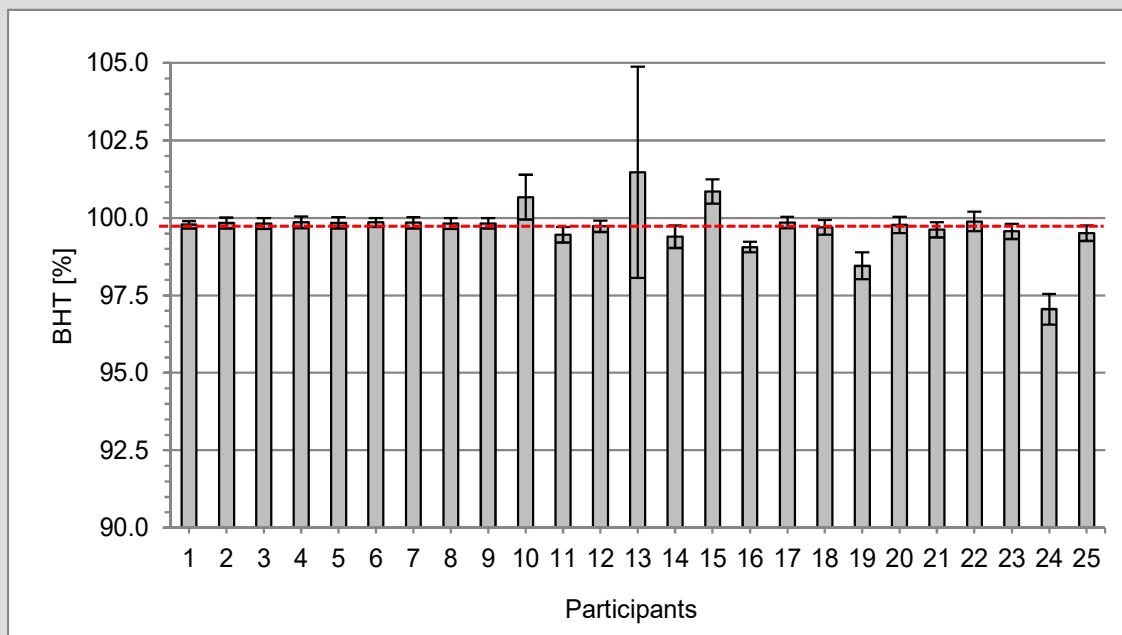


# Round Robin Test

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**Aim:** Performance of integration procedure



**Individual decision:**

- phase and baseline
- $^{13}\text{C}$  satellites
- appropriate signals

**Results:**

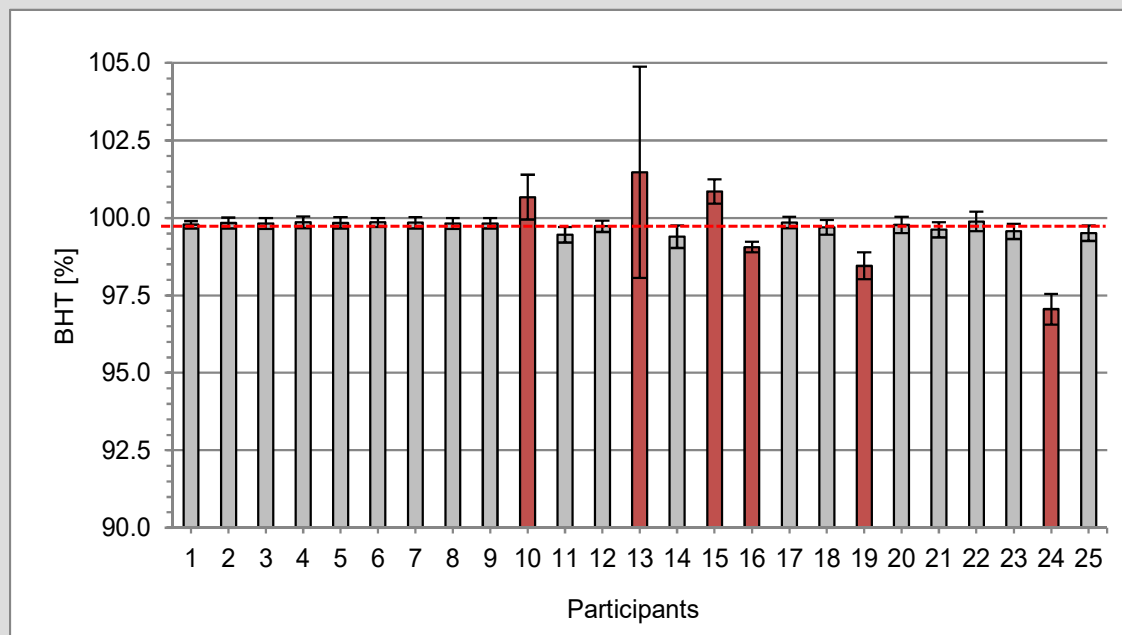
- content:  $99.7 \pm 0.3 \%$
- RSD  $\ll 1 \%$

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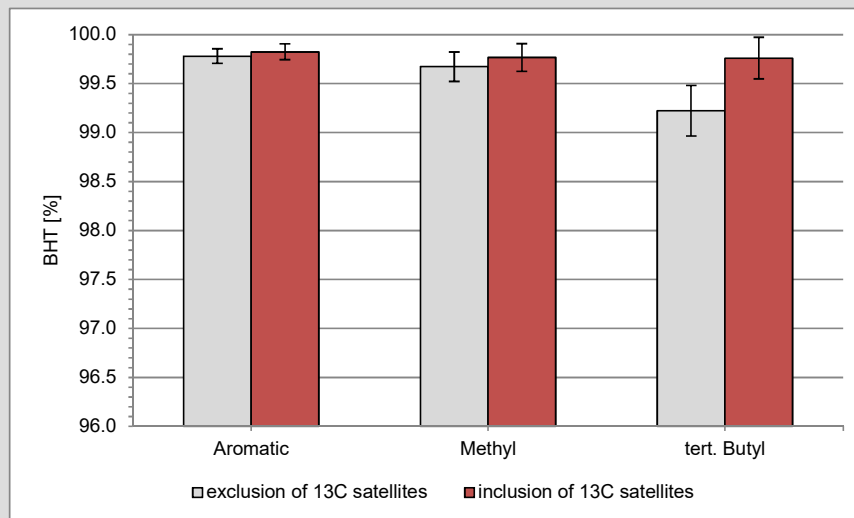
# Round Robin Test

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## Outliers:

- inadequate baseline correction
- **inadequate range of integration**  
→ exclusion of  $^{13}\text{C}$  satellites by integrating large and broad signals



# Round Robin Test Outlook

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- large number of publications on experimental design and parameter selection
- only a few publications about round robin tests and reproducibility

**Future projects:** Organisation of further round robin tests

- identification of possible pitfalls and stumbling blocks
- proof of competence towards authorities and customers

→ **increasing the acceptance of NMR as a valid quantitative method**