Deep Learning Based Phase and Baseline Correction

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Bruker Biospin

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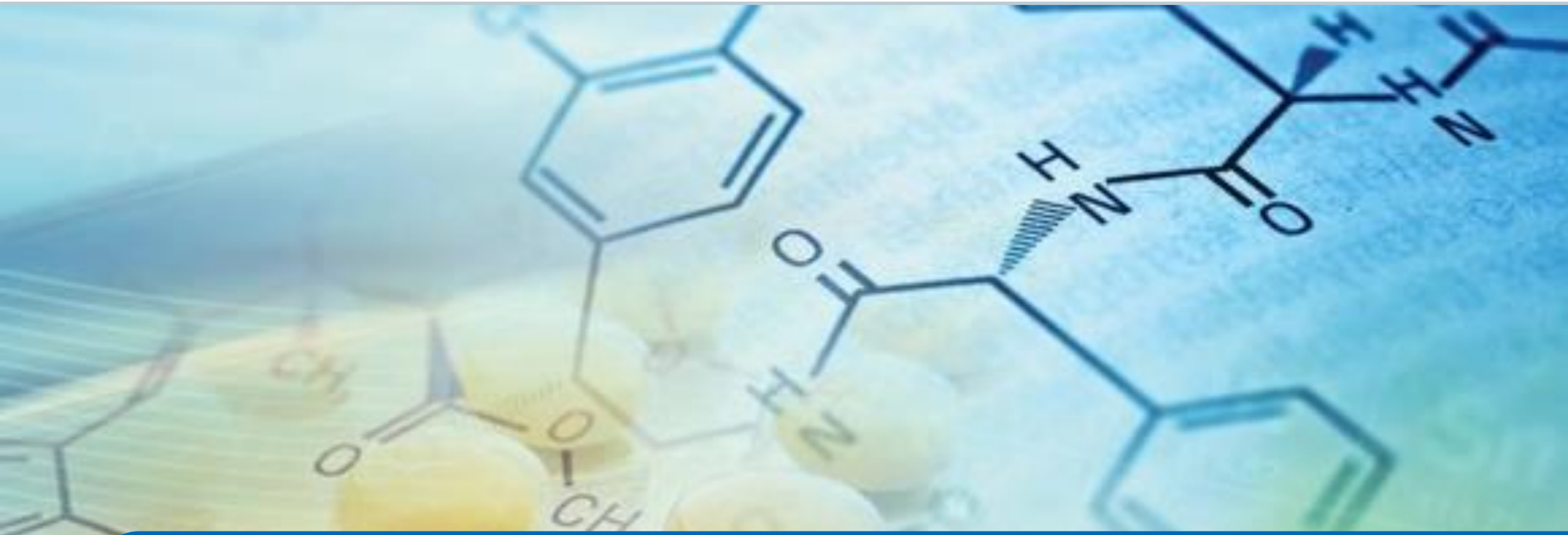


Machine Learning in NMR Spectroscopy

- The NMR community is increasingly using machine learning for the analysis of NMR spectra

Review and Prospect: Deep Learning in Nuclear Magnetic Resonance Spectroscopy

Dicheng Chen#[a], Zi Wang#[a], Di Guo[b], Vladislav Orekhov[c], Xiaobo Qu*[a]

Reconstruction of spectra from truncated free induction decays by deep learning in proton magnetic resonance spectroscopy

Hyochul Lee, Hyeong Hun Lee, Hyeonjin Kim

Accelerated Nuclear Magnetic Resonance Spectroscopy with Deep Learning

Xiaobo Qu[1*], Yihui Huang[1], Hengfa Lu[1], Tianyu Qiu[1], Di Guo[2], Tatiana Agback[3], Vladislav Orekhov[4], Zhong Chen[1*]

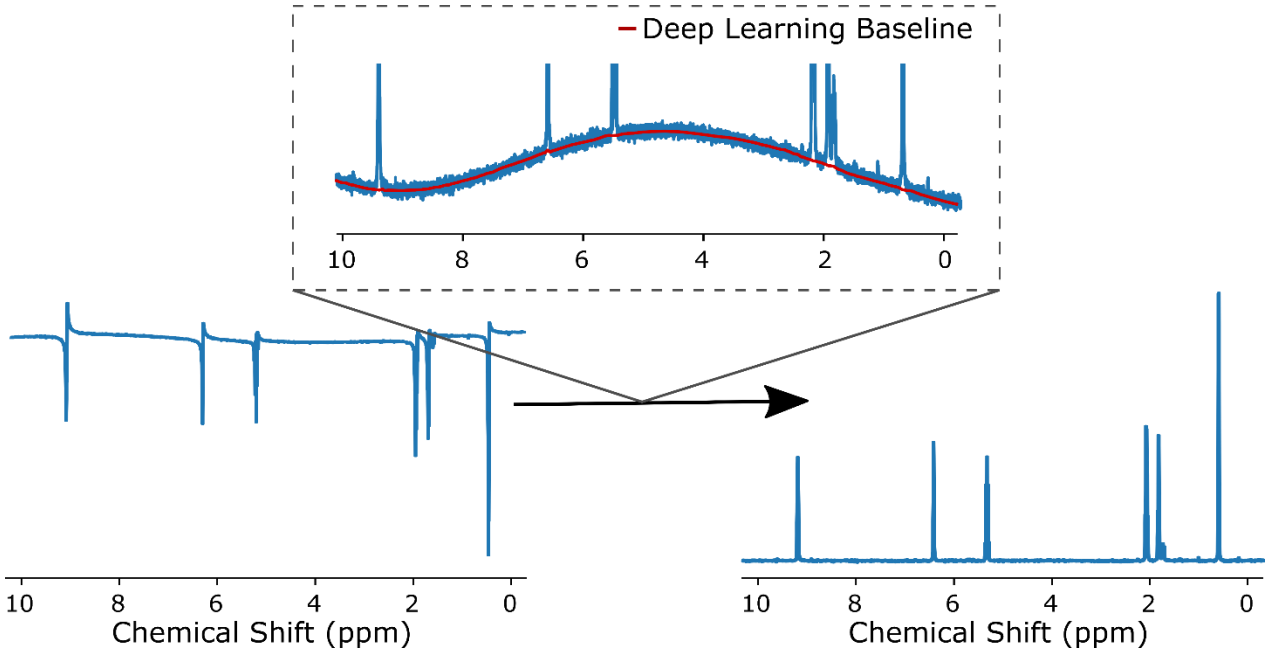
NMRNet: a deep learning approach to automated peak picking of protein NMR spectra.

Klukowski P[1], Augoff M[1], Zieba M[1], Drwal M[1], Gonczarek A[2,3], Walczak MJ[4,3].

- Bruker is part of it
  - Our latest application of deep learning has resulted in an improved phase and baseline correction algorithm for unsuppressed 1D ^{1}H NMR spectra

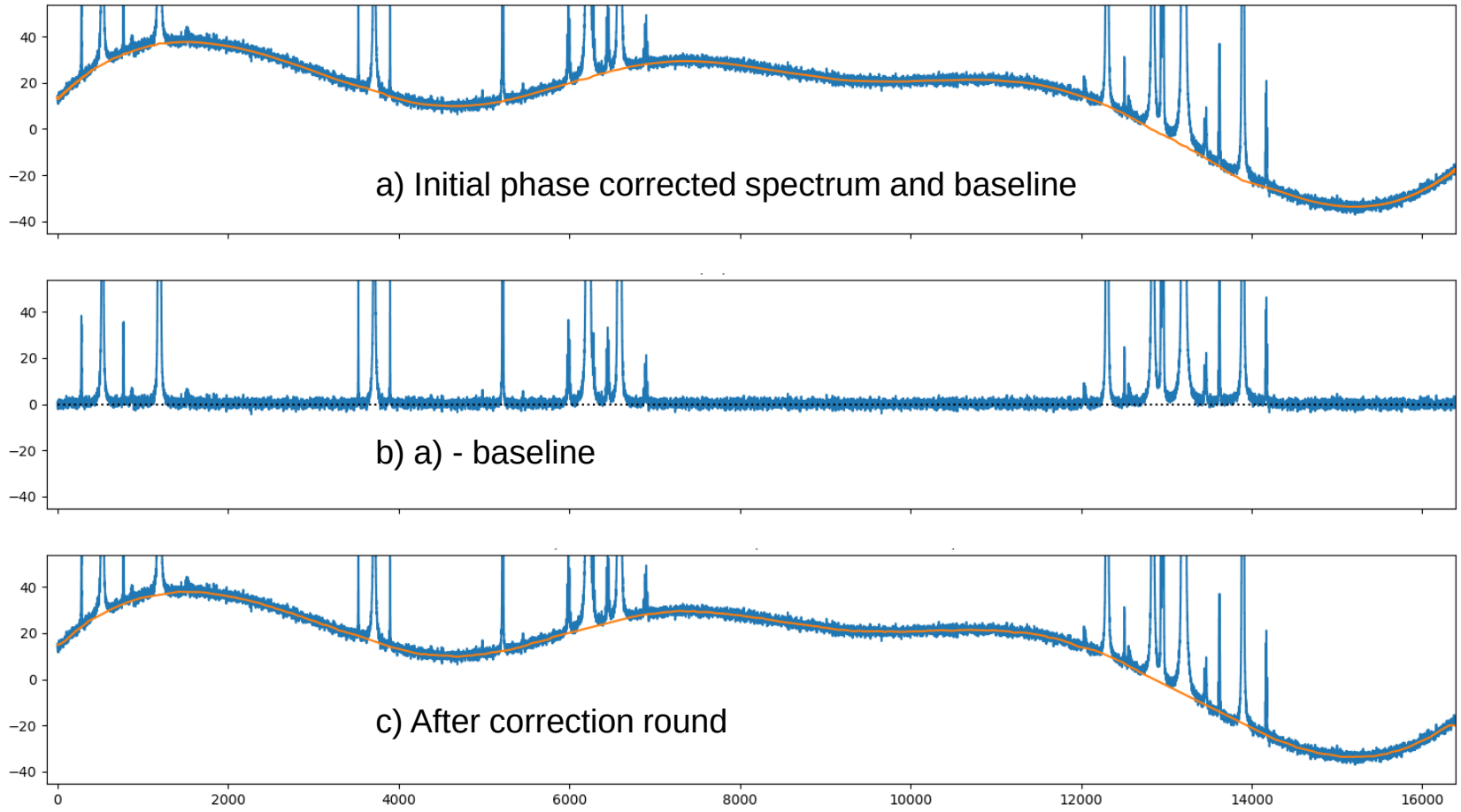
New *apbk* command for ^{1}H spectra

- We have developed a command for simultaneous phase and baseline correction of unsuppressed 1D 1H spectra
- The command is based on a deep learning algorithm for baseline detection



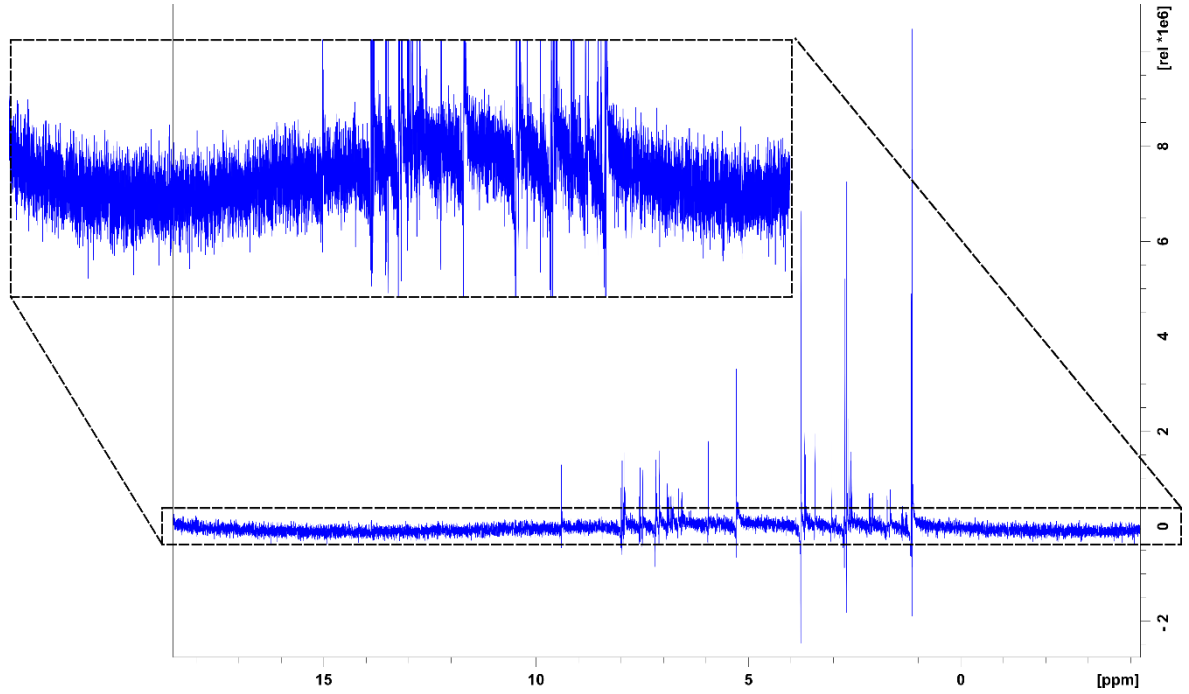
Methods

- Rough initial phase correction
- Neural network detects baseline
  - Convolutional recurrent network
  - Trained on synthetic data
- Iterative improvement of phase and baseline
  - Identify baseline regions
  - Perform phase fitting



Methods

- The neural network was trained using 100’000 artificially generated ^{1}H NMR spectra.

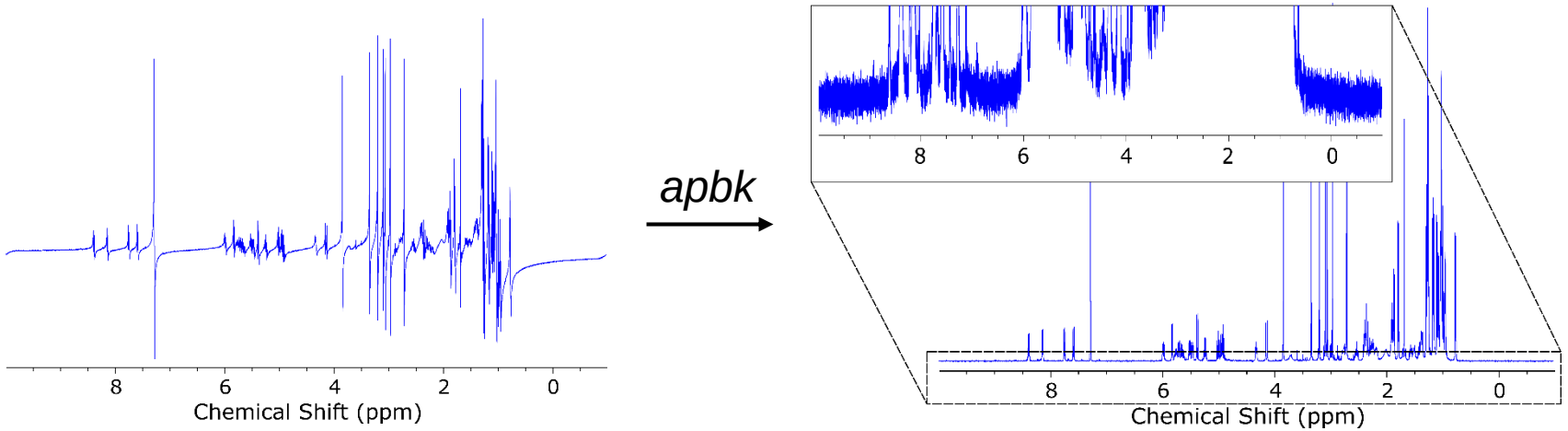


Training set parameters:

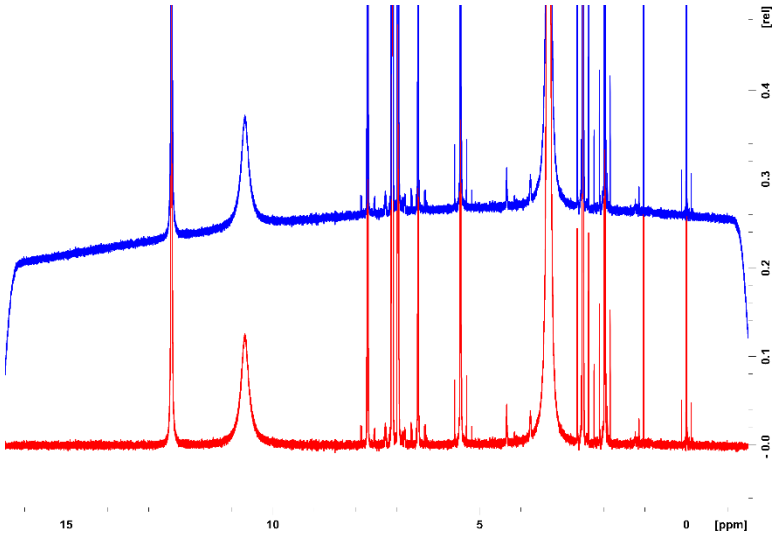
- 80 to 800 MHz base frequencies
- 10 to 10’000 SiNo
- Distribution of line widths, multiplicities, and J couplings that match typical experimental values
- Random phase and baseline distortion

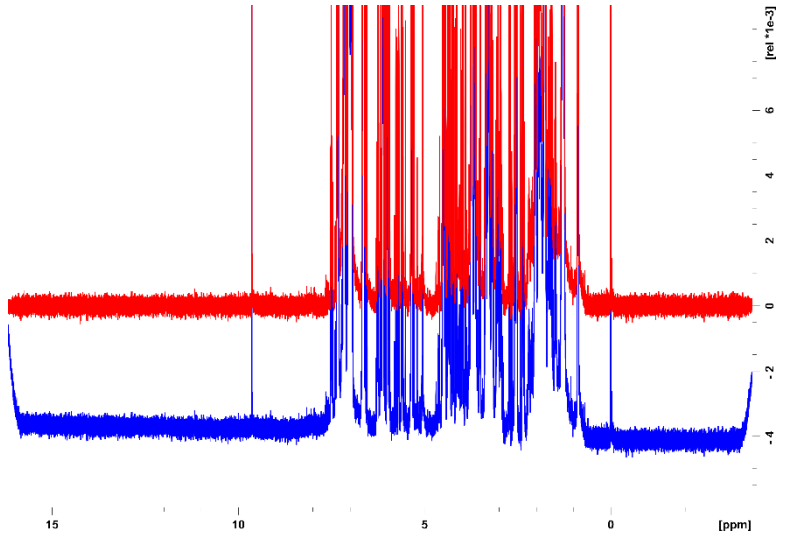
Results

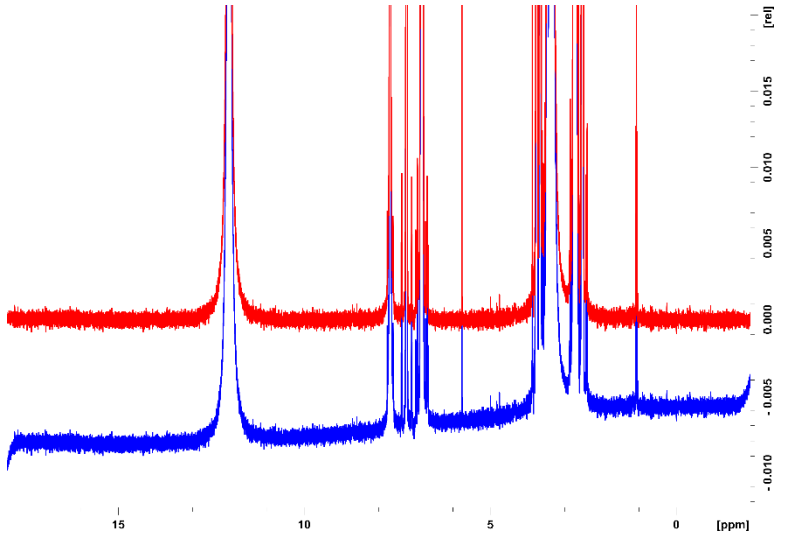
- The algorithm was tested against 100 experimental spectra that were phase and baseline corrected by NMR experts, and 1000 artificial spectra.
- It has shown overall **higher accuracy** than the commands for phase and baseline correction currently available in TopSpin (former *apbk –f* and *apk* + *abs*)
- It has also shown higher **robustness with respect to the base frequency**, providing excellent results also on data acquired with the Fourier 80



Results





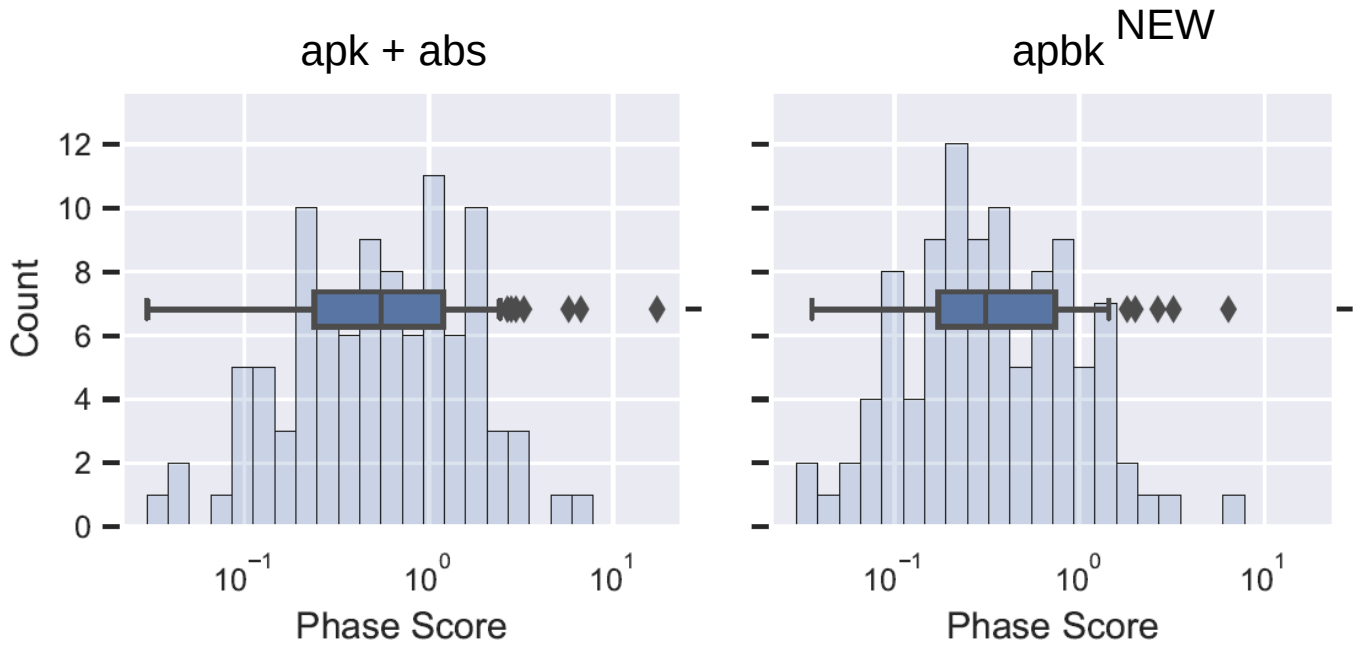


– Baseline only – *apbk* result

Results

Test on 100 experimental NMR spectra (80 MHz to 800 MHz)

Phase score
Corresponds to the average phase error of all peaks in a spectrum

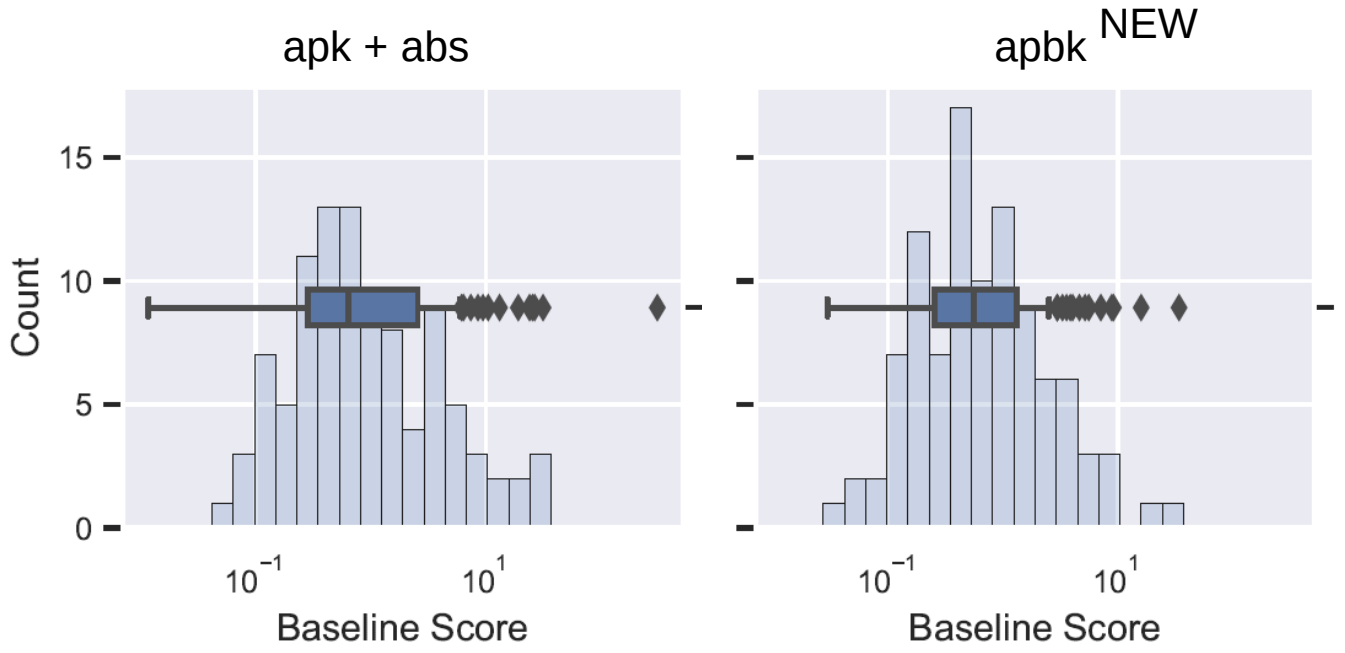


Q1	0.24°	**0.17°**
Median	0.55°	**0.31°**
Q3	1.19°	**0.64°**

Results

Test on 100 experimental NMR spectra (80 MHz to 800 MHz)

Baseline score
Corresponds to the z-score of the difference between real baseline and subtracted baseline with respect to the noise



Q1	0.28	**0.26**
Median	0.64	**0.51**
Q3	2.57	**1.34**

Release in TopSpin 4.1.2

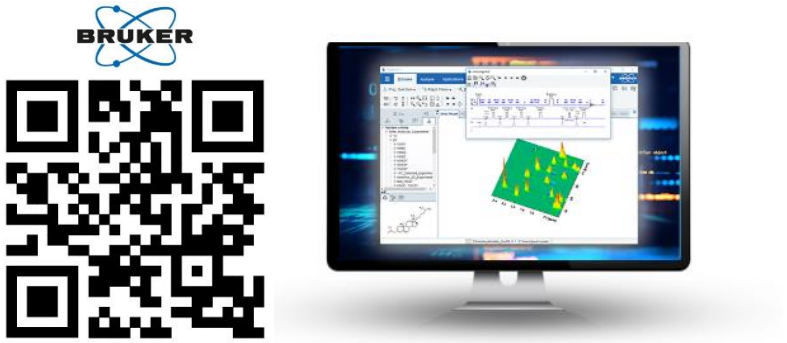
- The new apbk version optimized for unsuppressed ^{1}H spectra will be availabe with **TopSpin 4.1.2**
- Use this algorithm by typing *apbk* in the command line with ^{1}H 1D NMR dataset open
- Additional options

  apbk –po: performs phase correction only

  apbk –bo: performs baseline correction only

  apbk –intrng: uses user-defined integral regions

  apbk –apk0: optimize only PHC0 during phase correction



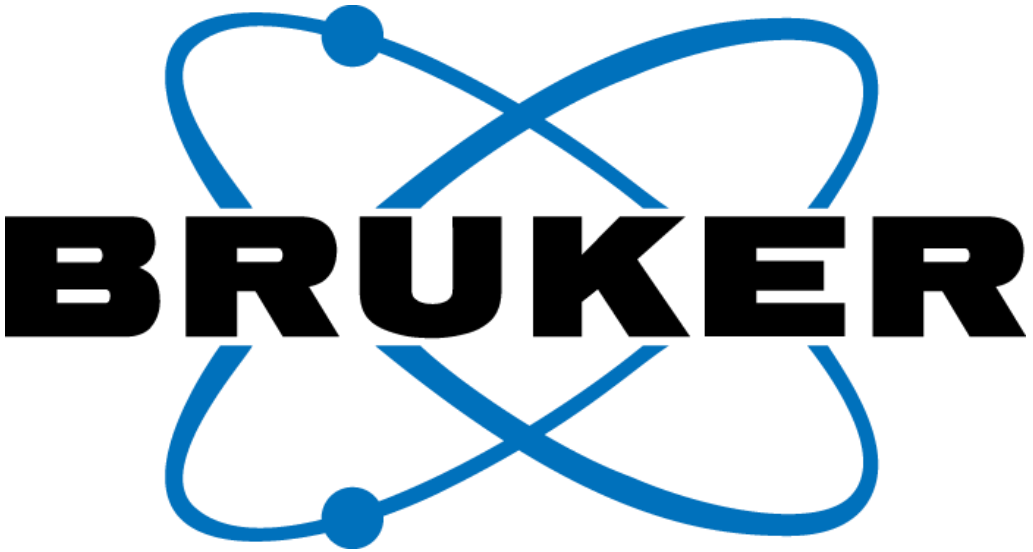
MAY 11, 2021

Deep Learning Based Phase and Baseline Correction on NMR Spectra

Bruker's commitment in developing artificial intelligence based NMR applications has led to a new function available in TopSpin: the automatic simultaneous phase and baseline correction of 1H NMR spectra.

Courious to learn more about it ?

Stay tuned for our webinar, coming on 11th May 4pm CET



Innovation with Integrity