

## NON-STATIONARY NMR SPECTROSCOPY

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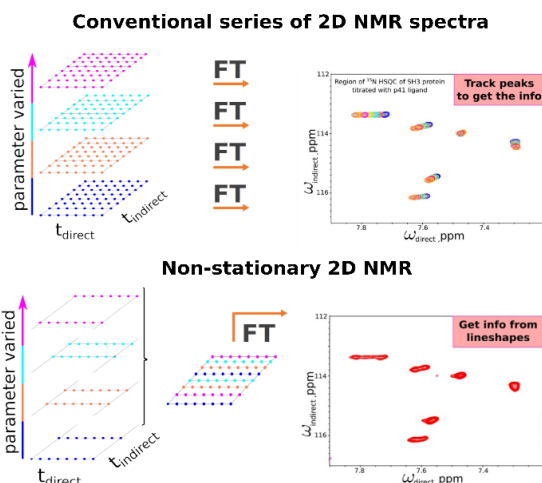
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The implicit assumption behind a routine NMR spectroscopy is that the parameters of an FID signal (frequencies, amplitudes, decay rates) are independent of time. NMR experiments, therefore, have to be performed under highly stable conditions. For example, the temperature has to be precisely controlled, and chemical reactions in the sample have to be avoided.

However, a series of NMR experiments with different environmental conditions is often used to monitor changes to molecular structure. For example, a series of spectra acquired at certain temperature values or ligand concentrations, changed from spectrum to spectrum, may be used to study temperature-induced protein unfolding.

My hypothesis, confirmed in several studies,<sup>[1–4]</sup> is that NMR experiments do not need to be conducted in a stable environment. The environmental conditions can be changed e.g. between the measurement of consecutive indirect dimension points. Such a *non-stationary signal* recorded for different temperatures, pH values, sample compositions and so on can actually replace a series of conventional spectra and be recorded in a time corresponding to the measurement of a single stationary spectrum.

In my presentation, I will summarize the recent progress and future plans in developing non-stationary NMR methods. I will discuss the possible applications in structural studies of large and small molecules, metabolomic screening and other fields.



### REFERENCES

- [1] Dass, R. et al., *Quick, sensitive serial NMR experiments with Radon transform*. *Journal of Magnetic Resonance* **2017**, *282*, 114–118. <https://doi.org/10.1016/j.jmr.2017.07.011>
- [2] Nawrocka, E.K. et al., *Nonstationary Two-Dimensional Nuclear Magnetic Resonance: A Method for Studying Reaction Mechanisms in Situ*. *Analytical Chemistry* **2019**, *91*(17), 11306–11315.
- [3] Romero, J. A. et al., *Non-Stationary Complementary Non-Uniform Sampling (NOSCO NUS) for Fast Acquisition of Serial 2D NMR Titration Data*. *Angewandte Chemie - International Edition* **2020**, *59*(52), 23496–23499.
- [4] Shchukina, A. et al., *Temperature as an Extra Dimension in Multidimensional Protein NMR Spectroscopy*. *Chemistry - A European Journal* **2021**, *27*(5), 1753–1767.