

SOME TIPS AND TRICKS FOR NMR METABOLOMICS AND LIPIDOMICS

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To date there are only two analytical techniques, namely, MS and NMR spectroscopy, which are suitable for large metabolomics and lipidomics screenings of various pathologies and for epidemiological studies. Metabolomics is currently a well-established topic both in education and in a wide range of research areas. Lipidomics has already provided new insights into health and disease monitoring. However, NMR lipidomics is much less explored in comparison with NMR metabolomics.

With the advent in NMR-based human phenotyping, as well as urine and plasma-based medical diagnosis and health status monitoring, several large groups have become well-established in NMR metabolomics. Recent studies have proven impressive interlaboratory reproducibility of NMR spectra when employing trained personnel and the latest industry standard solutions.^[1,2]

In addition to dedicated metabolomics groups, NMR metabolomics has penetrated many groups with nonexclusive or even marginal metabolomics interests. Our group is a good example where interests in various NMR topics coexist. We have also evaluated the NMR reproducibility for metabolomics in a "real-life" situation when combining both industry standard NMR solutions and multipurpose NMR equipment and we compared the reliability of NMR metabolomics data when involving both dedicated NMR operators and chemistry users from outside the NMR group.^[3]

The paper presents examples of NMR metabolomics and lipidomics applications in lifesciences. Some entry-level experimental tips and tricks are presented in order to ensure reliable NMR metabolomics and lipidomics data.

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REFERENCES

- [1] S. Monsonis Centelles, H. C. J. Hoefsloot, B. Khakimov, P. Ebrahimi, M. V. Lind, M. Kristensen, N. de Roo, D. M. Jacobs, J. van Duynhoven, C. Cannet, F. Fang, E. Humpfer, H. Schäfer, M. Spraul, S. B. Engelsen, A.K. Smilde, *Toward reliable lipoprotein particle predictions from NMR spectra of human blood: An interlaboratory ring test*, *Anal. Chem.* **2017**, *89*, 8004–8012.
<https://doi.org/10.1021/acs.analchem.7b01329>
- [2] B. Jiménez, E. Holmes, C. Heude, R.F. Tolson, N. Harvey, S.L. Lodge, A.J. Chetwynd, C. Cannet, F. Fang, J. T. M. Pearce, M.R. Lewis, M.R. Viant, J.C. Lindon, M. Spraul, H. Schaefer, J.K. Nicholson, *Quantitative lipoprotein subclass and low molecular weight metabolite analysis in human serum and plasma by ¹H NMR spectroscopy in a multilaboratory trial*, *Anal. Chem.* **2018**, *90*, 11962–11971.
<https://doi.org/10.1021/acs.analchem.8b02412>
- [3] C. Stavarache, A. Nicolescu, C. Duduianu, G.L. Ailisei, M. Balan-Porcărașu, M. Cristea, A.-M. Macsim, O. Popa, C. Stavarache, A. Hîrtopeanu, L. Barbeș, R. Stan, H. Iovu, C. Deleanu, *A real-life reproducibility assessment for NMR metabolomics*, *Diagnostics* **2022**, *12*, 559.
<https://doi.org/10.3390/diagnostics12030559>