



**TOP**

**SPEC**



Horizon 2020

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# **TopSpec**

## **Project Deliverable Report**

### **D8.5 TopSpec Scientific reports and publications**

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**Internal reviewers:** -

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**Lead beneficiary:** MS

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## VERSION AND CONTROLS

Version	Date	Reason	Editor/ Author/ Reviewer
1.0	14 Dec 2022	First release	Jan Commandeur

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# 1 Background

Scientific results of the TopSpec project were to be communicated to the scientific community through open access articles in scientific journals. Here we present a list of articles published so far.

## 2 List of Scientific Publications

### 2.1 Peer-reviewed articles:

Data processing:

[Monitoring glycation levels of a bispecific monoclonal antibody at subunit level by ultrahigh-resolution MALDI FT-ICR mass spectrometry. Gstottner C, Reusch D, Habegger M, Dragan I, Van Veelen P, Kilgour DPA, et al. MAbs. 2020;12\(1\):1682403.](#)

Exploration of state-of-the-art antibody analysis:

[Interlaboratory Study for Characterizing Monoclonal Antibodies by Top-Down and Middle-Down Mass Spectrometry. Srzentic K, Fornelli L, Tsybin YO, Loo JA, Seckler H, Agar JN, et al. J Am Soc Mass Spectrom. 2020;31\(9\):1783-802.](#)

Data processing:

[Transient-Mediated Simulations of FTMS Isotopic Distributions and Mass Spectra to Guide Experiment Design and Data Analysis, Nagornov KO, Kozhinov AN, Gasilova N, Menin L, Tsybin YO. J Am Soc Mass Spectrom. 2020;31\(9\):1927-42.](#)

Orbitrap™ acquisition methods:

[Exploring frontiers of orbitrap performance for long transients, Denisov E, Damoc E, Makarov A. Int J Mass Spectrom. 2021;466.](#)

Data processing:

[Drug-to-Antibody Ratio Estimation via Proteoform Peak Integration in the Analysis of Antibody–Oligonucleotide Conjugates with Orbitrap Fourier Transform Massspectrometry, Nagornov KO, Gasilova N, Kozhinov AN, Virta P, Holm P, Menin L, et al. Anal Chem. 2021;93\(38\):12930-7.](#)

Initiative to define the human proteome:

[The Human Proteoform Project: Defining the human proteome, Smith LM, Agar JN, Chamot-Rooke J, Danis PO, Ge Y, Loo JA, et al., Sci Adv. 2021;7\(46\):eabk0734.](#)

Method development for top-down proteomics:

[TDFragMapper: a visualization tool for evaluating experimental parameters in top-down proteomics, Dhenin J, Lima DB, Dupre M, Chamot-Rooke J. Bioinformatics. 2021;38\(4\):1136-8.](#)

ETD for top-down and middle-down analysis of antibodies:

[Structural Analysis of Monoclonal Antibodies with Top-down and Middle-down Electron Transfer Dissociation Mass Spectrometry: The First Decade, Fornelli L, Ayoub D, Srzentic K, Nagornov KO, Kozhinov AN, Gasilova N, et al. Chimia. 2022;76\(1-2\):114-26.](#)

## 2.2 Other:

Orbitrap instrument development:

[A Novel Family of Quadrupole-Orbitrap Mass Spectrometers for a Broad Range of Analytical Applications, Preprints.org, 08 Jun 2020](#)

TopSpec project overview:

[Zubarev, R. \(2022\) 'Next-generation precision antibody profiling; from science fiction to reality', Project Repository Journal., 15, pp. 38-41.](#)

New analysis tool for charge state determination in complex datasets:

[Adding colour to mass spectra: Charge Determination Analysis \(CHARDA\) assigns charge state to every ion peak, ChemRxiv, 17 Sept 2021](#)

## 2.3 Software:

Improved assignment algorithms for antibody spectra that will be used for TopSpec:

[C. Gstöttner, D. Reusch, M. Habegger, I. Dragan, P. van Veelen, D.P.A. Kilgour, Y.O. Tsybin, Y.E.M. van der Burgt, M. Wuhrer & S. Nicolardi \(2019\): Monitoring glycation levels of a bispecific monoclonal antibody at subunit level by ultrahigh resolution MALDI FT-ICR mass spectrometry.](#)

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