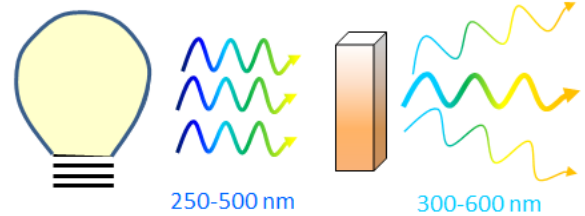
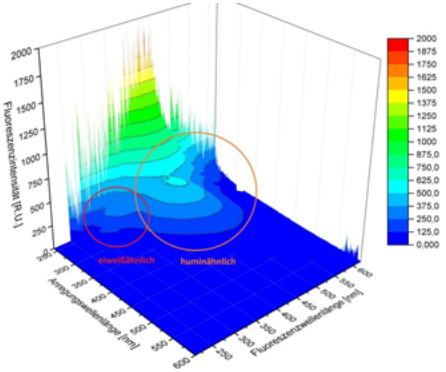
Friedrich-Schiller-Universität Jena

seit 1558

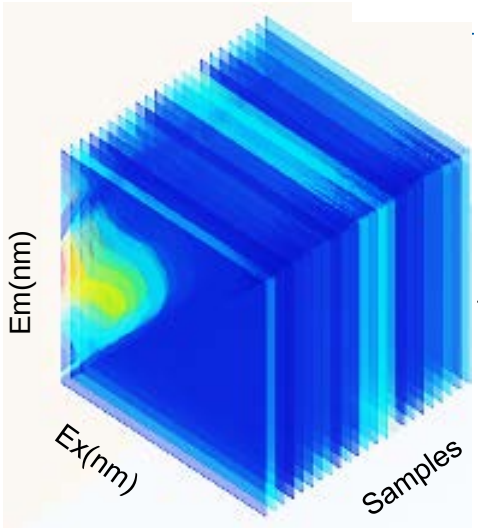
DBU

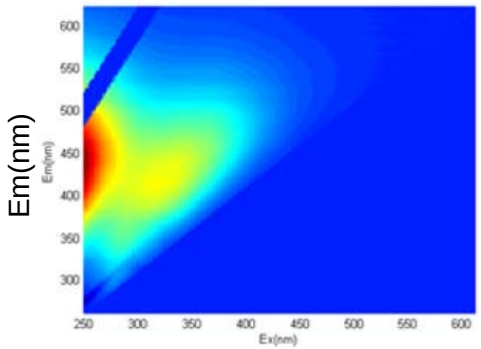
Deutsche Bundesstiftung Umwelt

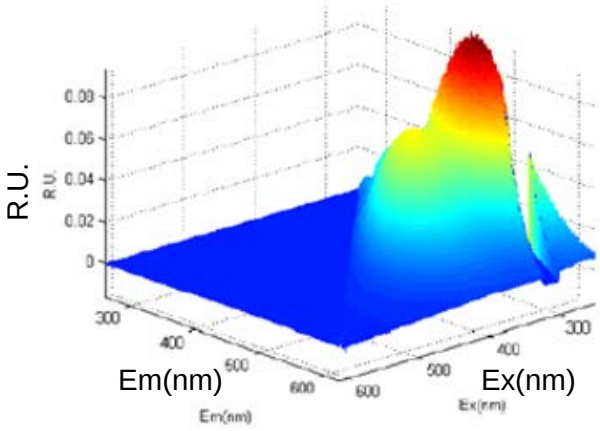




Anregungs-Fluoreszenzspektrum







PARAFAC modelling and FT-ICR-MS data from Muldenberg reservoir samples for better description of the DOM composition for drinking water treatment

Christin Wilske, Peter Herzsprung, Jürgen. W. Einax, Wolf von Tümpling

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Red Mulde in the catchment area of the Muldenberg dam

Picture of Herrn Dr. Herzsprung, Helmholtz-Zentrum für Umweltforschung - UFZ

Red Mulde in the catchment area of the Muldenberg dam

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Would you like to drink this water?

Red Mulde in the catchment area of the Muldenberg dam

Picture of Herrn Dr. Herzsprung, Helmholtz-Zentrum für Umweltforschung - UFZ

Would you like to drink this water?

What is responsible for the yellow-brownish color of the water?

Red Mulde in the catchment area of the Muldenberg dam

Picture of Herrn Dr. Herzsprung, Helmholtz-Zentrum für Umweltforschung - UFZ

Would you like to drink this water?

What is responsible for the yellow-brownish color of the water?

Which influence have the humic acids on the drinking water quality?

Red Mulde in the catchment area of the Muldenberg dam

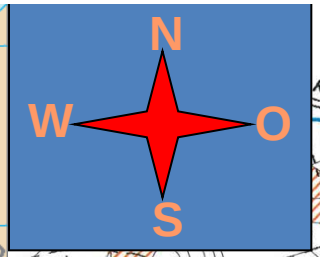
Picture of Herrn Dr. Herzsprung, Helmholtz-Zentrum für Umweltforschung - UFZ

Would you like to drink this water?

What is responsible for the yellow-brownish color of the water?

Which influence have the humic acids on the drinking water quality?

What effort is required to produce drinking water?



Outflow
TSP

Saubach
SBA

Sauteich
STE

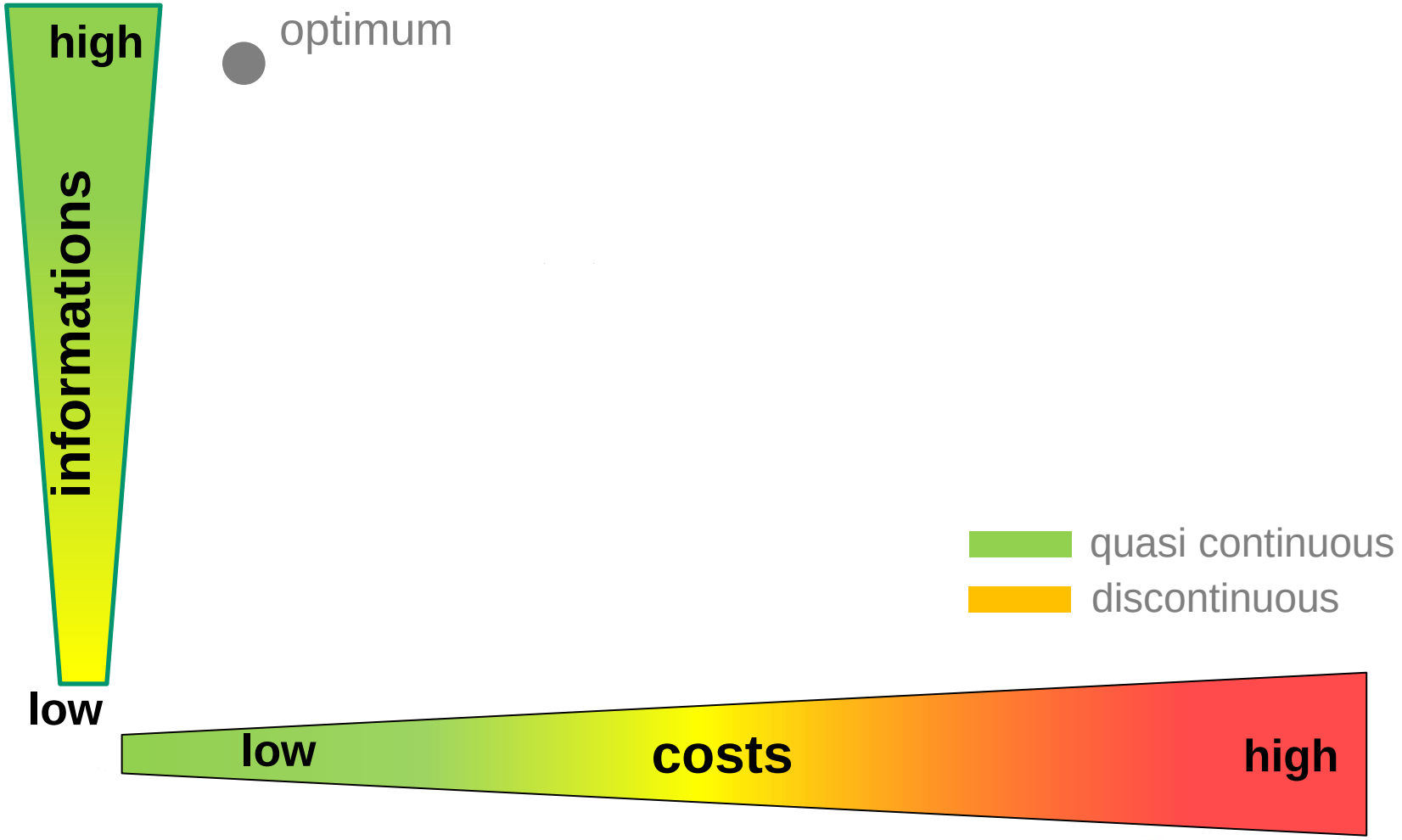
Red Mulde
RMU

White Mulde
WMU

1 km

_muld_ae_flaeche.shp

Comparison of the analytical methods



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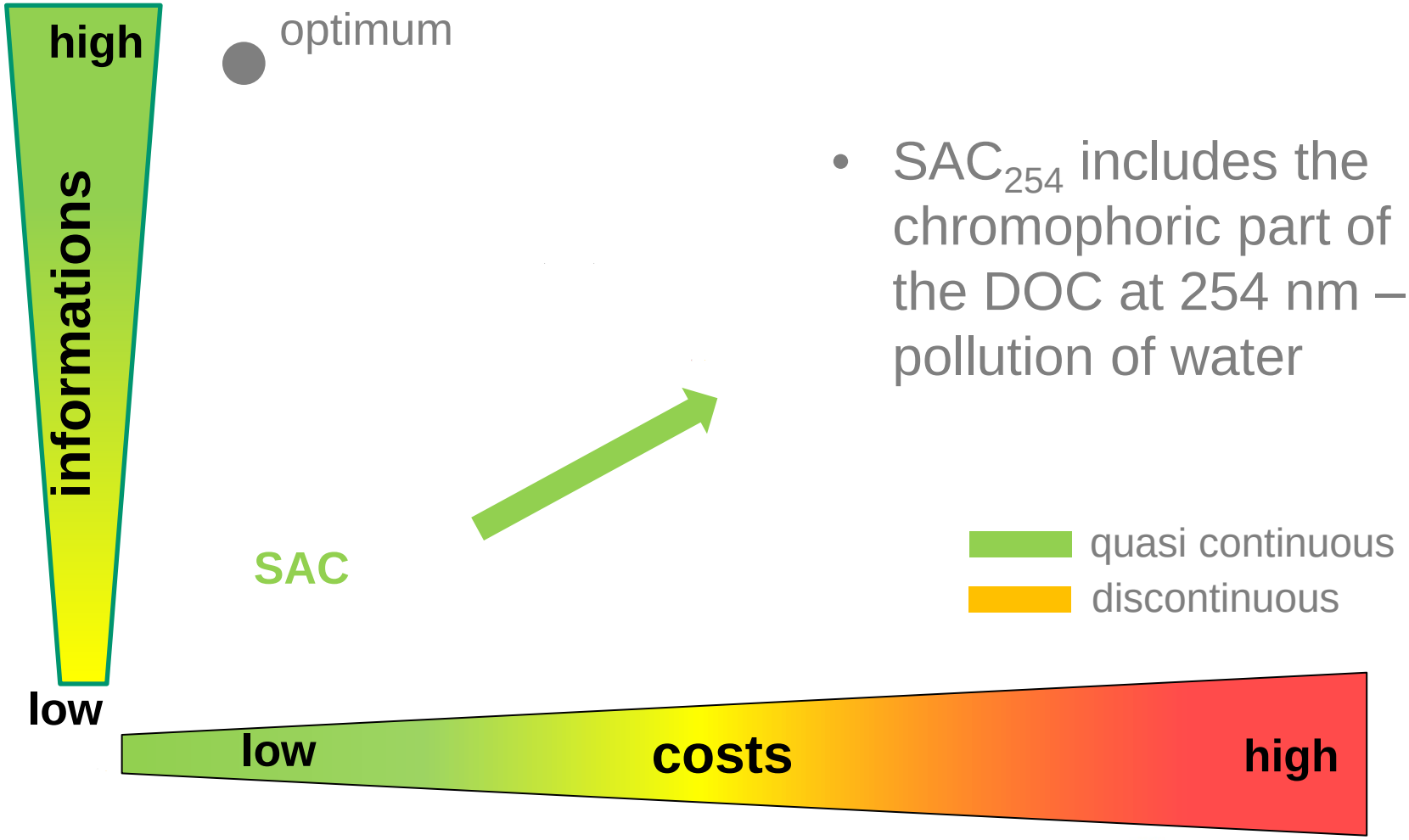
Comparison of the analytical methods



- SAC_{254} includes the chromophoric part of the DOC at 254 nm – pollution of water

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Comparison of the analytical methods

optimum

- determination of DOC as a sum parameter with IR-spectrometry – pollution of water

DOC

quasi continuous
discontinuous

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Comparison of the analytical methods

optimum

LC-OCD

- component wise characterization of DOM – e. g. HS I und HS II or Building Blocks

quasi continuous
discontinuous

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Comparison of the analytical methods

optimum

FT-ICR-MS

- mass spectrometry for characterization of DOM (different substances)

quasi continuous
discontinuous

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Comparison of the analytical methods

optimum

3D-fluorescence spectroscopy

- low-cost
- quasi continuous
- much more information
- minimal sample preparation

quasi continuous
discontinuous

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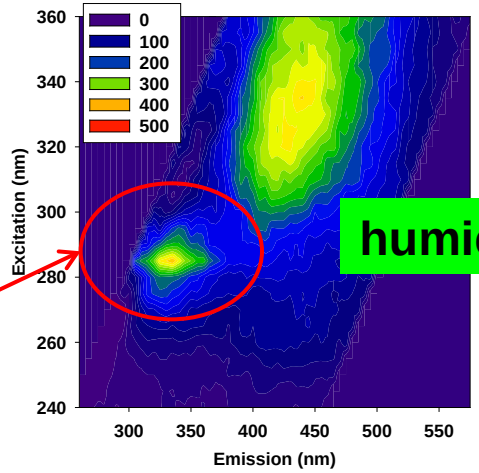
Separation of protein-like and humic-like fluorescence

water sample

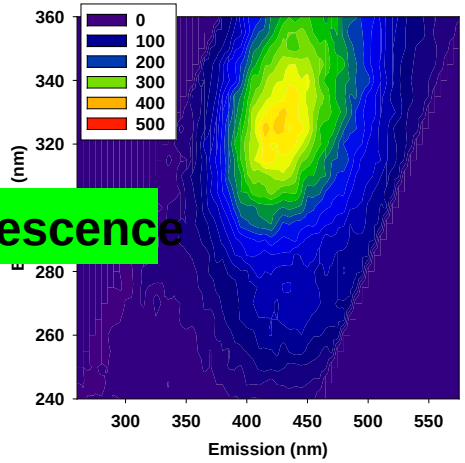
direct measurement

0,2 µm filtration

STE Konzentrat unfiltered



STE Konzentrat filtered



protein-like fluorescence

humic-like fluorescence

Enrichment of bacteria

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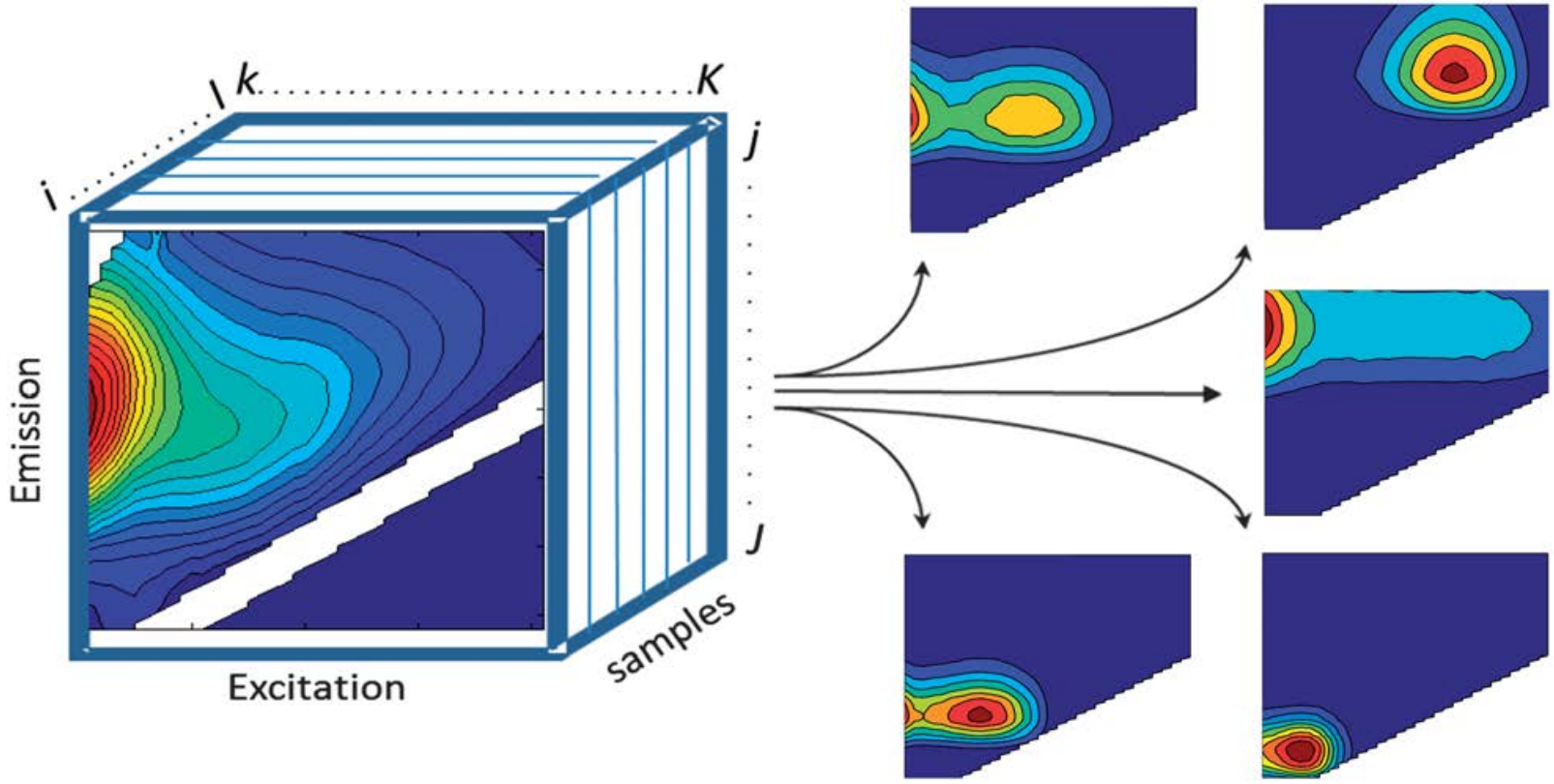
Parallel Factor Analysis (PARAFAC) – decomposition of components



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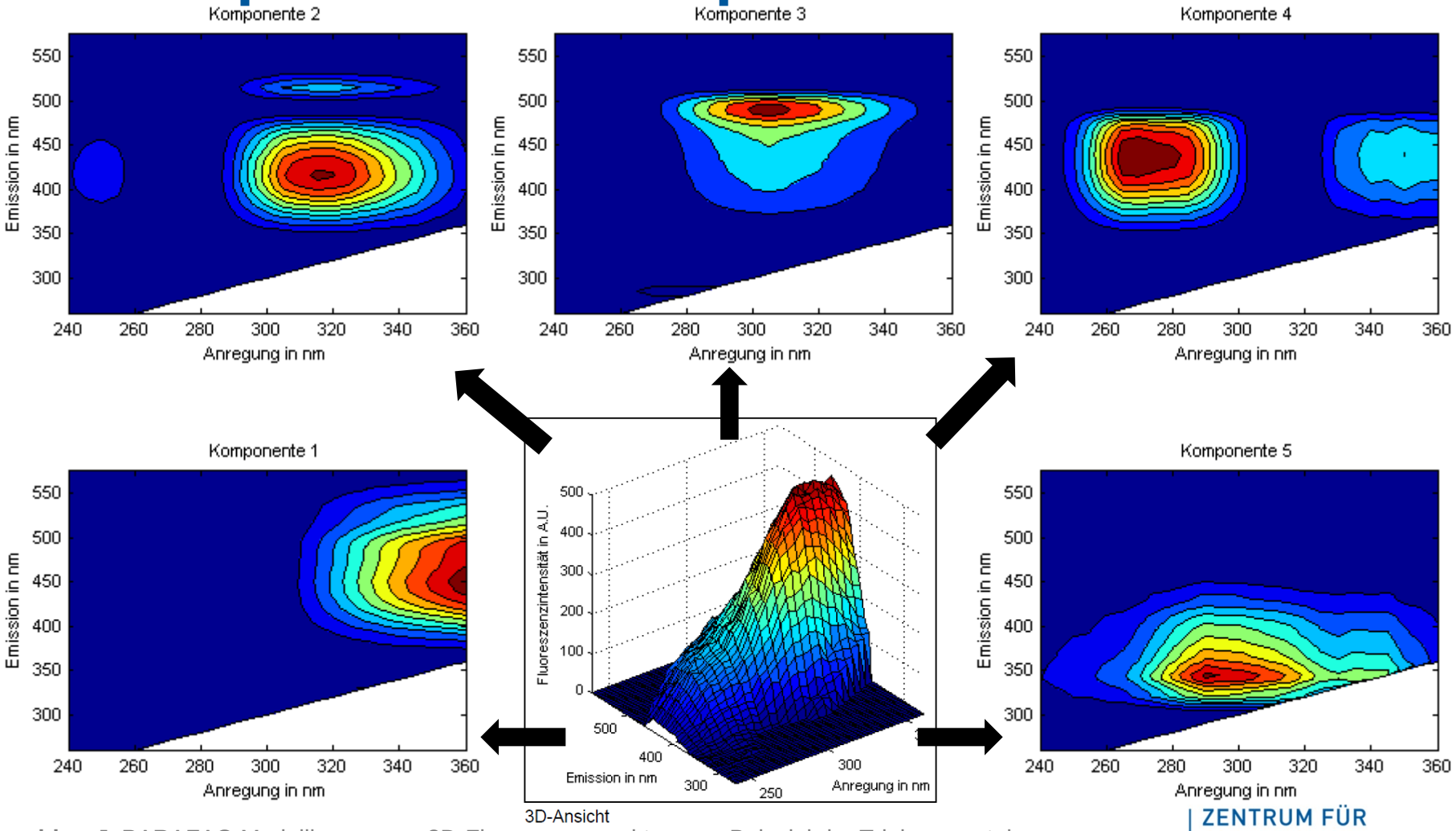
Parallel Factor Analysis (PARAFAC) – decomposition of components



Bravidor, J. PARAFAC-Modellierung von 3D-Fluoreszenzspektren am Beispiel der Trinkwassertalsperre Muldenberg - Eine Möglichkeit der DOC-Charakterisierung. 2011. Diplomarbeit.

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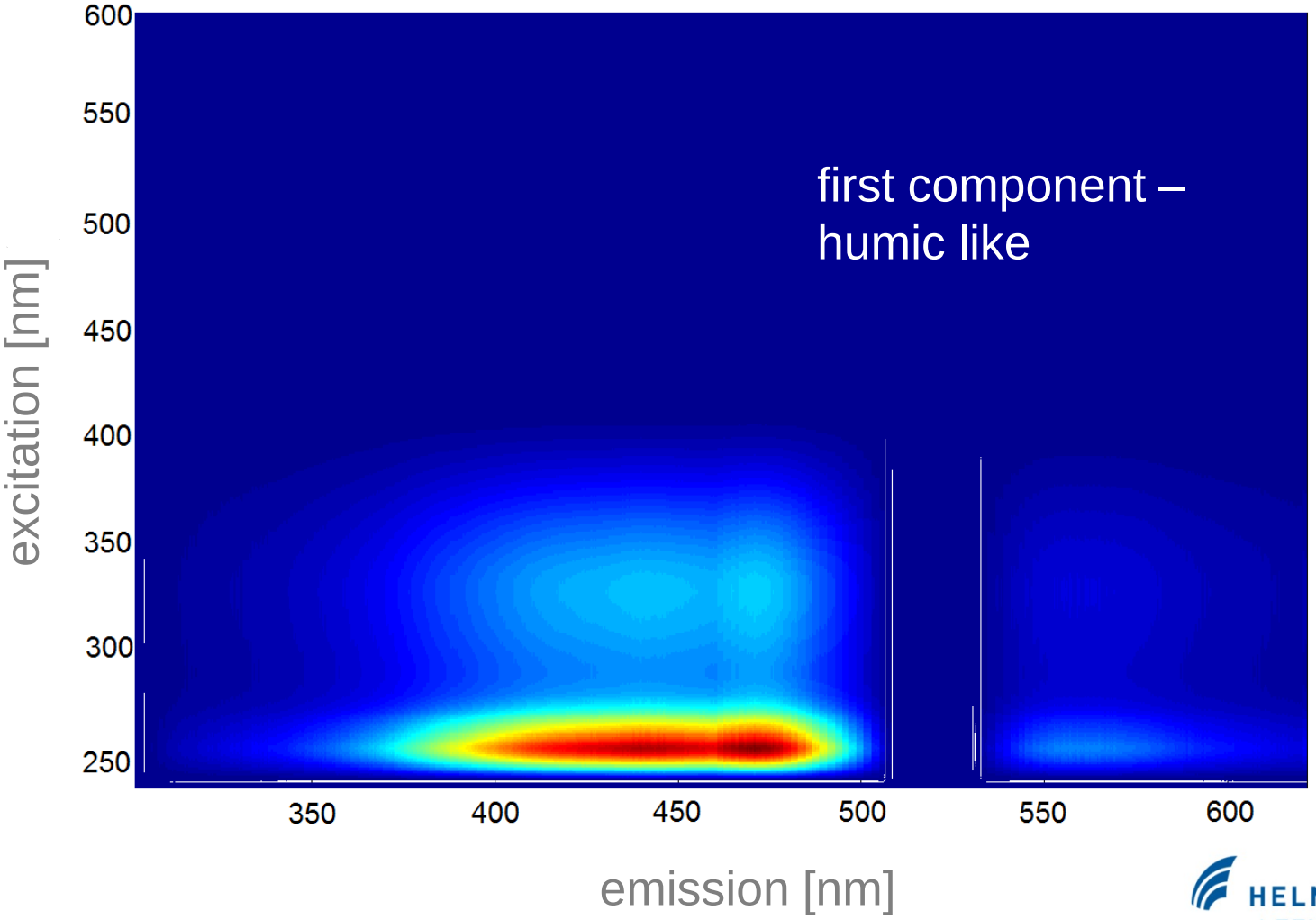
PARAFAC model of the Muldenberg dam and the catchment area

First PARAFAC results:

- Three component model of all samples during winter from October to February

- Two component model of all samples over the year 2016

Three component model



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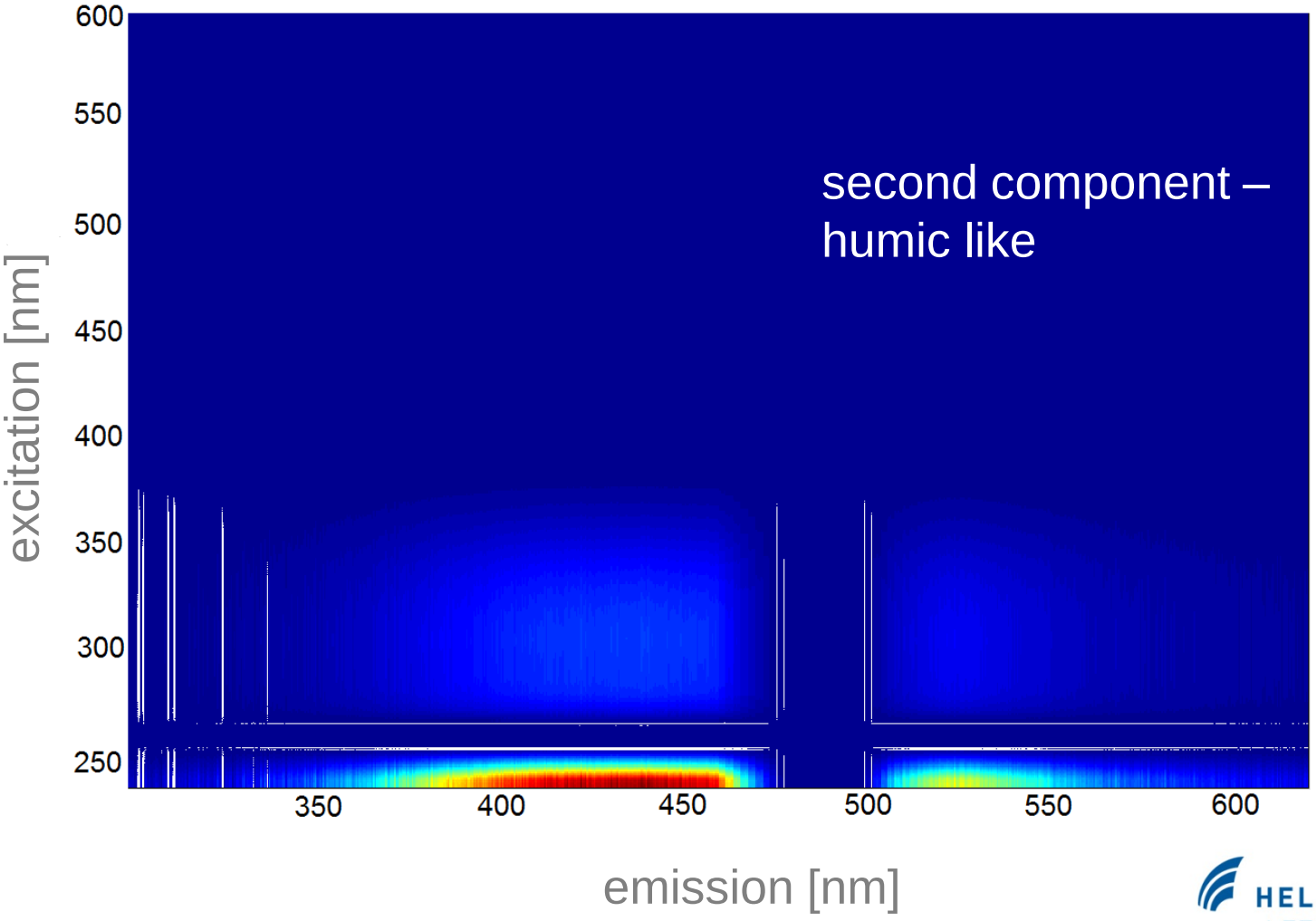
Three component model



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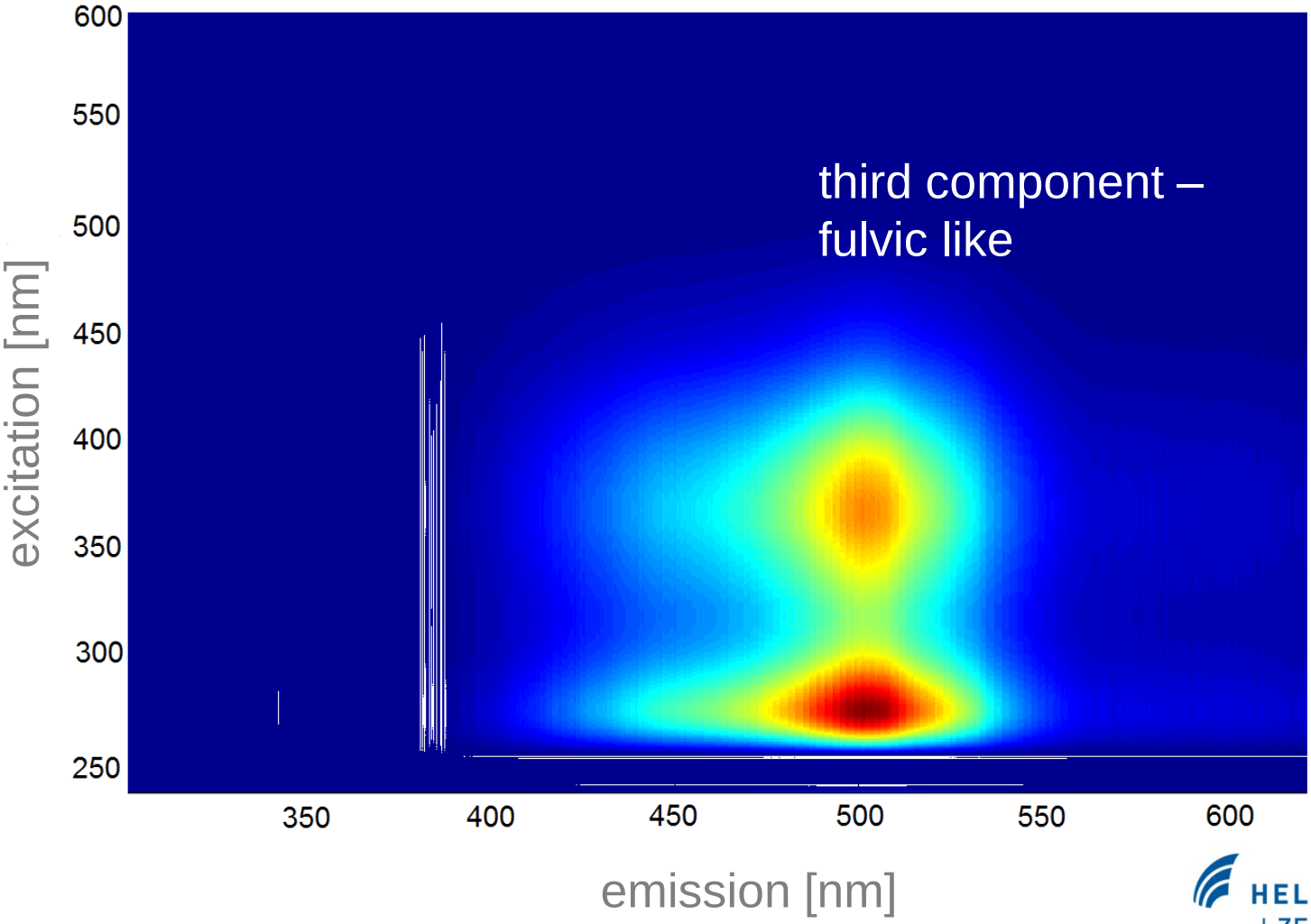
Three component model



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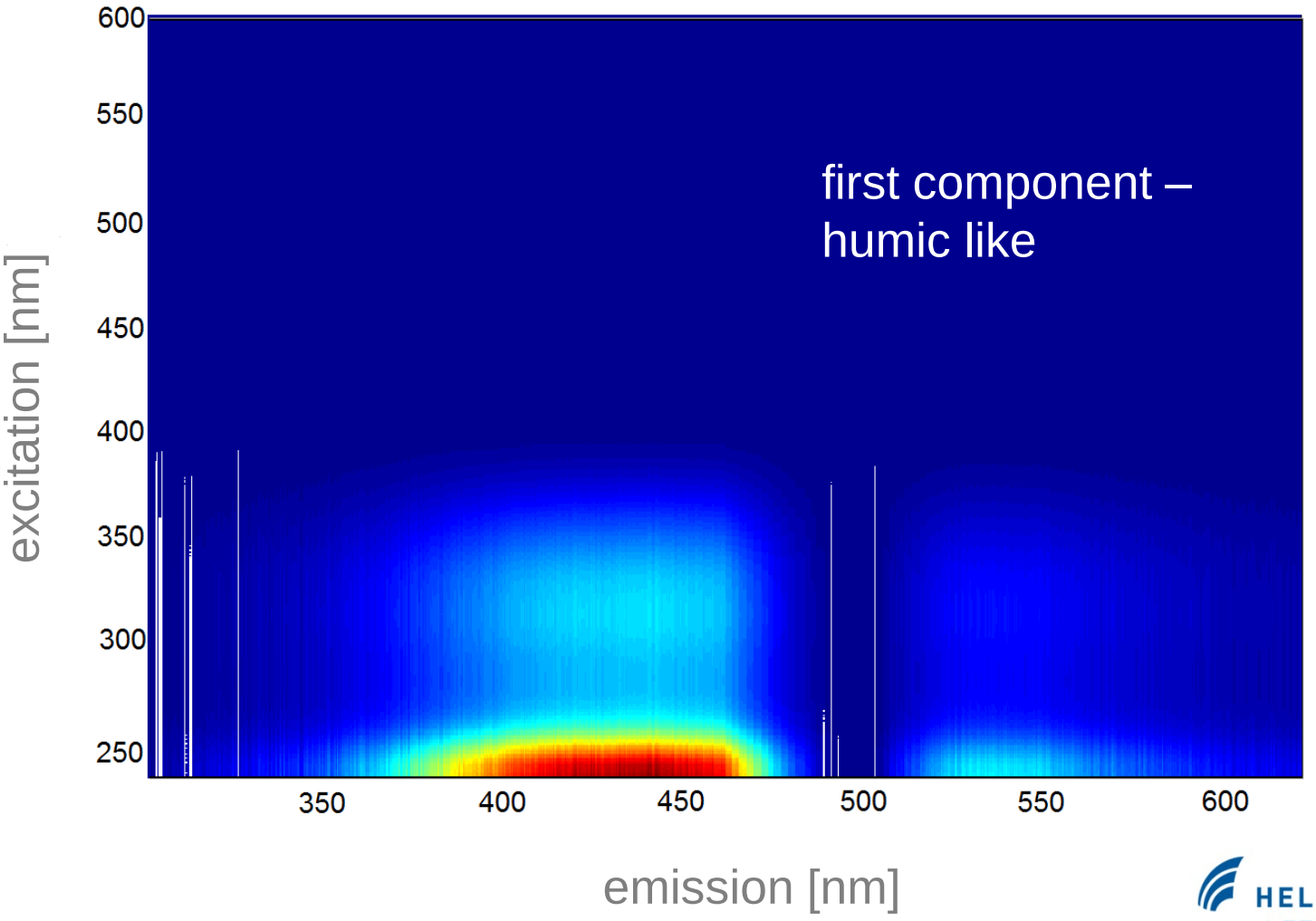
Two component model



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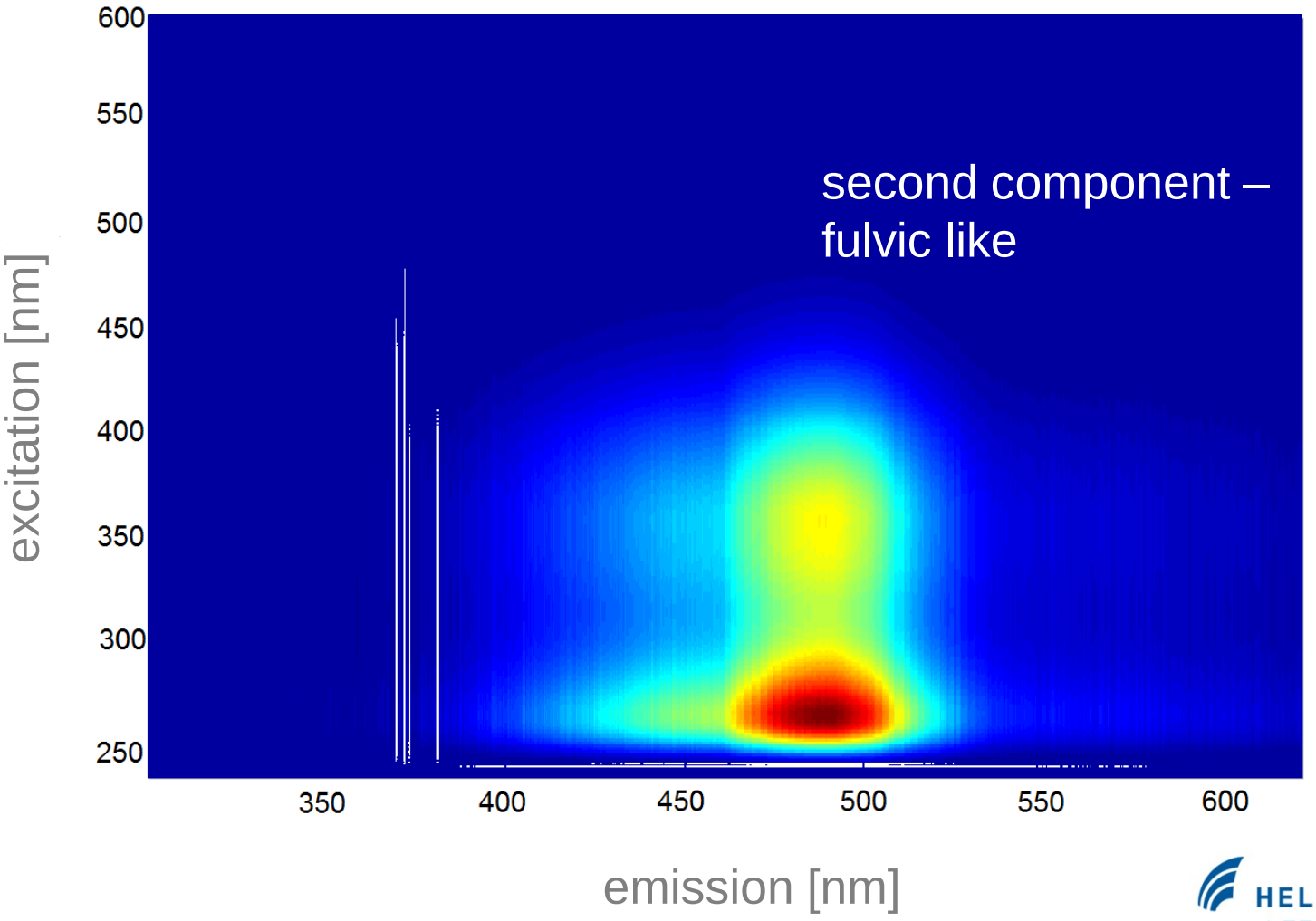
Two component model



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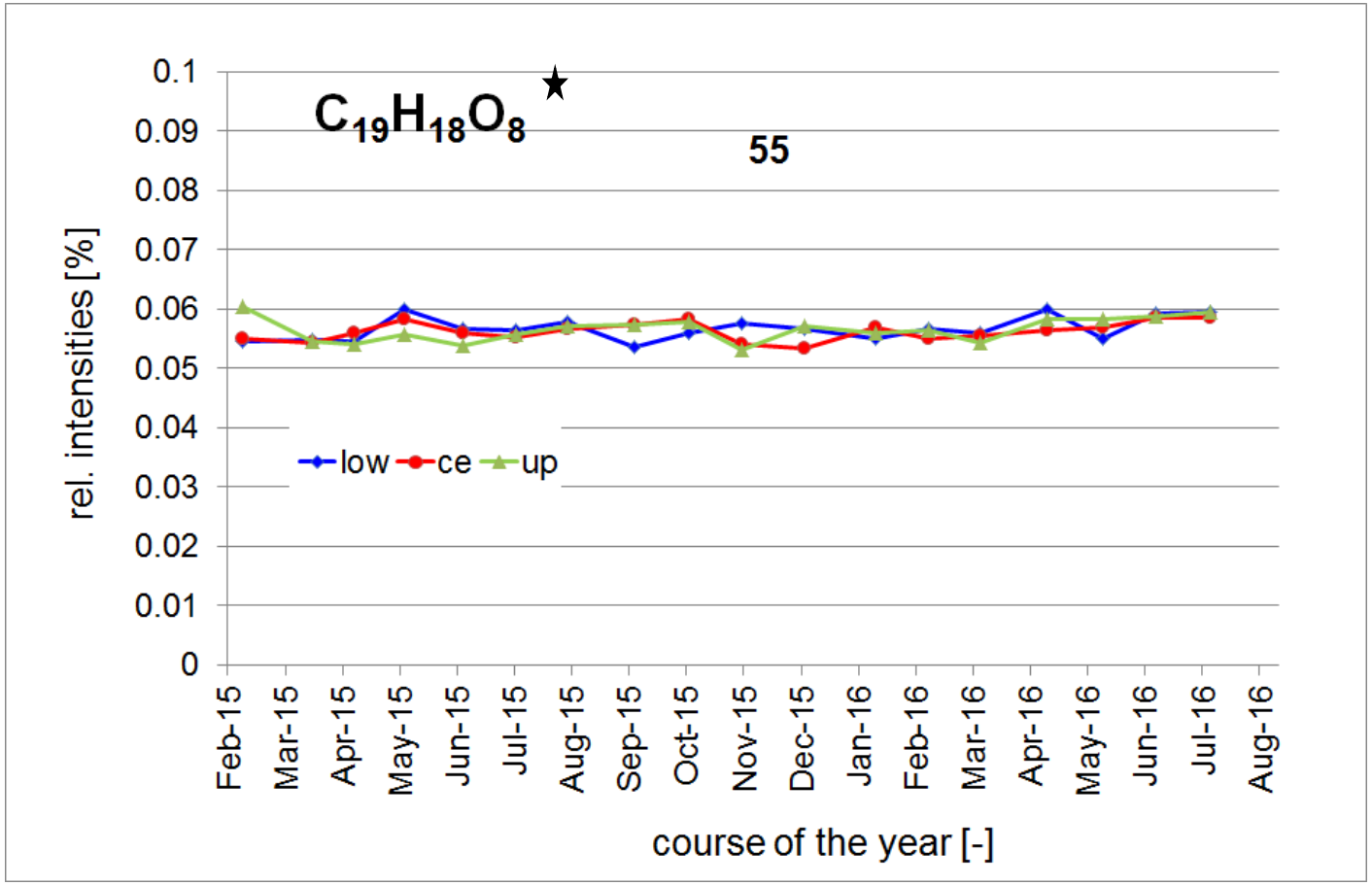
Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR-MS)



- selected according to minimum intensity variance

★ component found in 55 samples (total common presence)

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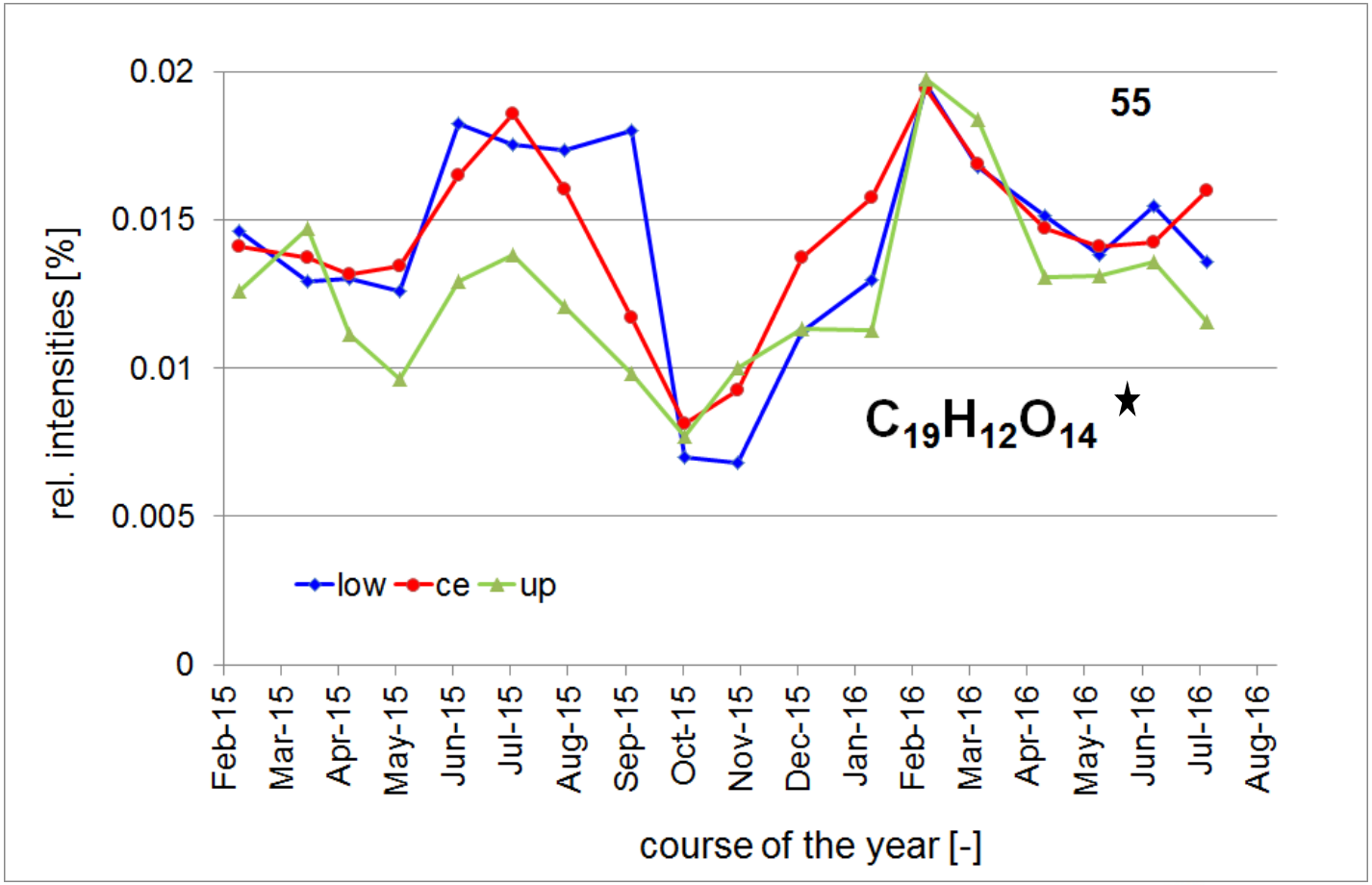
Fourier-transform ion cyclotron resonance mass spectrometry (FT-ICR-MS)



★component found in 55 samples (total common presence)

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Conclusion

i) During winter month a three component model and during the year 2016 a two component model was performed

ii) Three component model: first and second component are humic like and the third component is fulvic like

iii) Two component model: first component is humic like and the second one is fulvic like

iv) The isomer mixture with the formula $C_{19}H_{18}O_8$ shows mainly the same level of percentage intensity in all depths and months

v) The isomer mixture with the formula $C_{19}H_{12}O_{14}$ shows significant annual differences and partly as function of depth

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Outlook

- Characterization of components in the reservoirs of 2016/2017
  - further PARAFAC
  - further mass spectrometry (FT-ICR-MS) measurements
- Correlations between PARAFAC components and other analytical parameters
- Evaluation of the photochemical experiment (August 2018)
- Investigations during extreme rainfall or spring thaw with the help of an online fluorescence sensor of Moldaenke in 2019

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Thanks for your Attention

PD Dr. Wolf von Tümpling, Dr. Peter Herzsprung, Prof. Dr. Jürgen W. Einax, Prof. Dr. Georg Pohnert, GEWANA, LTV, DBU (Hr. Stock)

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