



BRNOFACULTYUNIVERSITYOF CHEMISTRYOF TECHNOLOGY



Humeomics fractionation – a molecular zoom in natural organic matter





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Humeomics origins...







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Basis of a Humeomics Science: Chemical Fractionation and Molecular Characterization of Humic Biosuprastructures

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Supporting Information

ABSTRACT: We propose a mild stepwise fractionation of molecular components of a humic acid (HA) suprastructure and their structural identification by advanced analytical methods. This procedure may be the basis of a "Humeomics" approach to characterize natural humic molecules and clarify their relations with ecosystems functions. Sequential fractionation included: (1) organic solvent extraction, (2) transesterification with boron trifluoride in methanol (BF₃-CH₃OH), (3) methanolic alkaline hydrolysis (KOH-CH₂OH), and (4) cleavage of ether and glycosidic bonds with HI





Humeomics origins...

















Aims of my internship



- 1. creation/recreation of cooperation
 - erasmus+ projects for students
 - projects (SOMOPRO) •
- 2. educational aims
 - familiarization with new methods







Napolitan experiences





















Napolitan experiences?!!













Humeomics fractionation (HSS







ARTICLE

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Occluded water



Humeomics fractionation (HSS



- chemical fractionation authors <u>A. Nebbioso</u>, A. Piccolo (HA) M. Drosos (NOM – mainly SOM)
- proper reagents HA structure is cleaved relatively small molecules are released => separation on water- and organosoluble fractions
- reason/aim:
 - decrease of polydispersity => better characterization
 - better comparison of effects of applied chemicals, humics according to their source, place, isolation procedure...





Scheme of procedure







Humeomics fractionation (HSS



1. step (labile fraction)

- AQU1 (using 0,1 M HCl) only for NOM; in the case of HA not obtained
- ORG1 (dichloromethane in MeOH 2:1)

2. step (weakly bound esters)

- 12% BF₃ in MeOH transesterification with BF₃–MeOH Biosuprastructure
- L/L extraction = water/chloroform => AQU2/ORG2

3. step (strongly bound esters)

- 1M KOH v MeOH methanolic alkaline hydrolysis
- L/L extraction = water/ dichloromethane
 => AQU3/ORG3

4. step (etheric bonds)

- 47% HI etheric and glycosidic bonds cleavage=>AQU4
- Rest material extracted with diethylether => ORG4

RESOM

 – alkaline extraction of residual organic matter + comparison with NOM extracted directly from source material



Occluded water



Humeomics fractionation (HSS



methods necessary for characterization of individual fractions:

- AQU fractions:
 - mass yields
 - elemental analysis
 - FTIR
 - NMR
 - LC-MS
- ORG fractions:
 - mass yields
 - elemental analysis
 - FTIR
 - NMR
 - GC-MS







My humeomics research



Humeomics fractionation done on samples:

1. Chernozem soil + comparison with soils already analyzed => classical procedure of humeomics fractionation

2. Identification of way of interaction of heavy metals on NOM





My humeomics research



metals interaction with OM – gravimetric results





My humeomics research



metals interaction with NOM – FTIR





My humeomics research



Brno University of Technology

chernozem – gravimetric results





Future/Possibilities



data processing => publication

- \rightarrow NMR data (liquid-state)
- \rightarrow LC MS (samples waiting for analysis)
- \rightarrow GC-MS (waiting for data processing)



introducing the humeomics on BUT, Faculty of chemistry

- \rightarrow bachelor thesis
- \rightarrow project (GAČR, COST...)

cooperation with you ...

- \rightarrow humeomics can reveal influence of different added substances on NOM
- \rightarrow vice vestra can help to identify where/how these added substances interact with NOM
- \rightarrow fate of carbon (14C labelled) etc..



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Thank you for your attention!!!

