

Supporting Information

Exploring ionic liquid-biomass interactions: Towards the improved isolation of shikimic acid for star anise pods

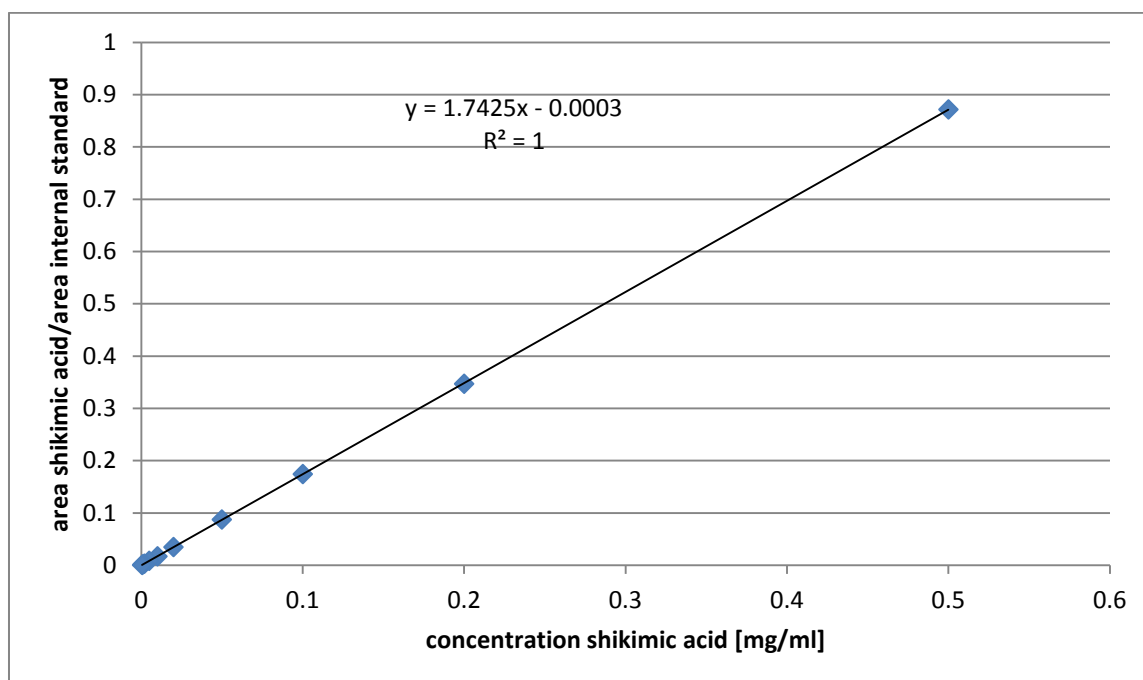
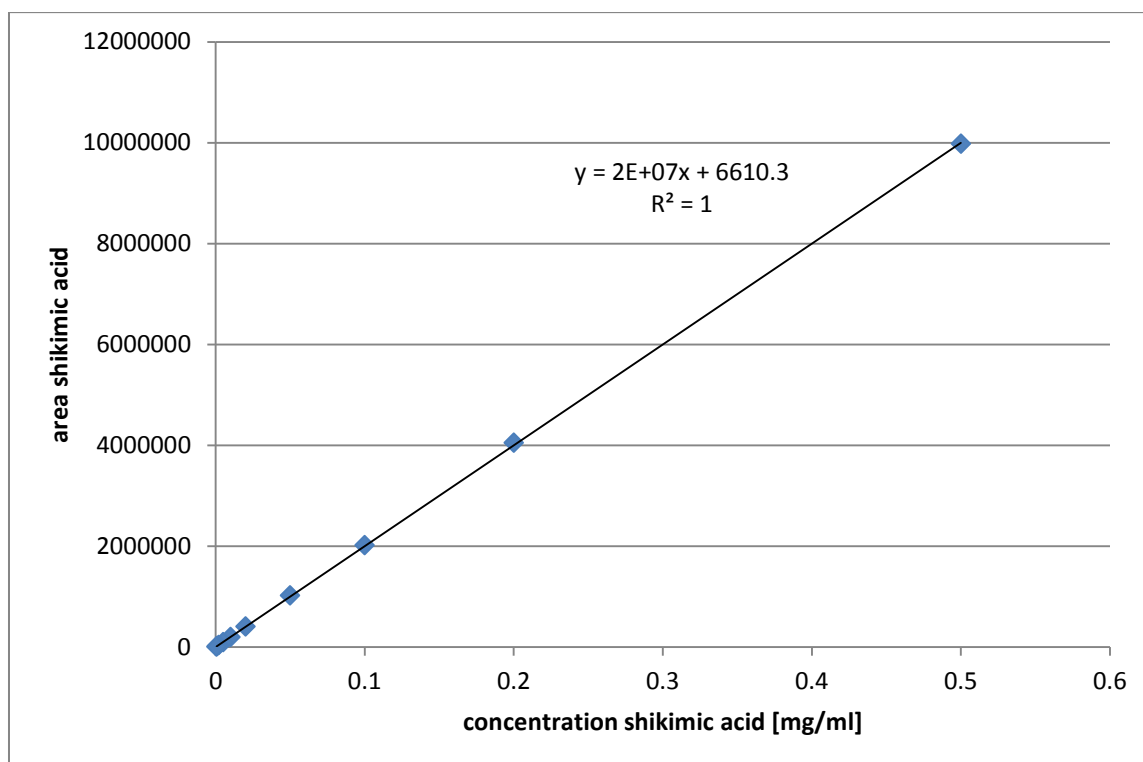
Ronald Zirbs,^a Katharina Strassl,^b Peter Gaertner,^b Christian Schröder,^{*c} and Katharina Bica^{*b}

^a *Group for Biologically Inspired Materials, Institute of Nanobiotechnology (DNBT), University of Natural Resources and Life Sciences, Muthgasse 11, 1190 Vienna, Austria.*

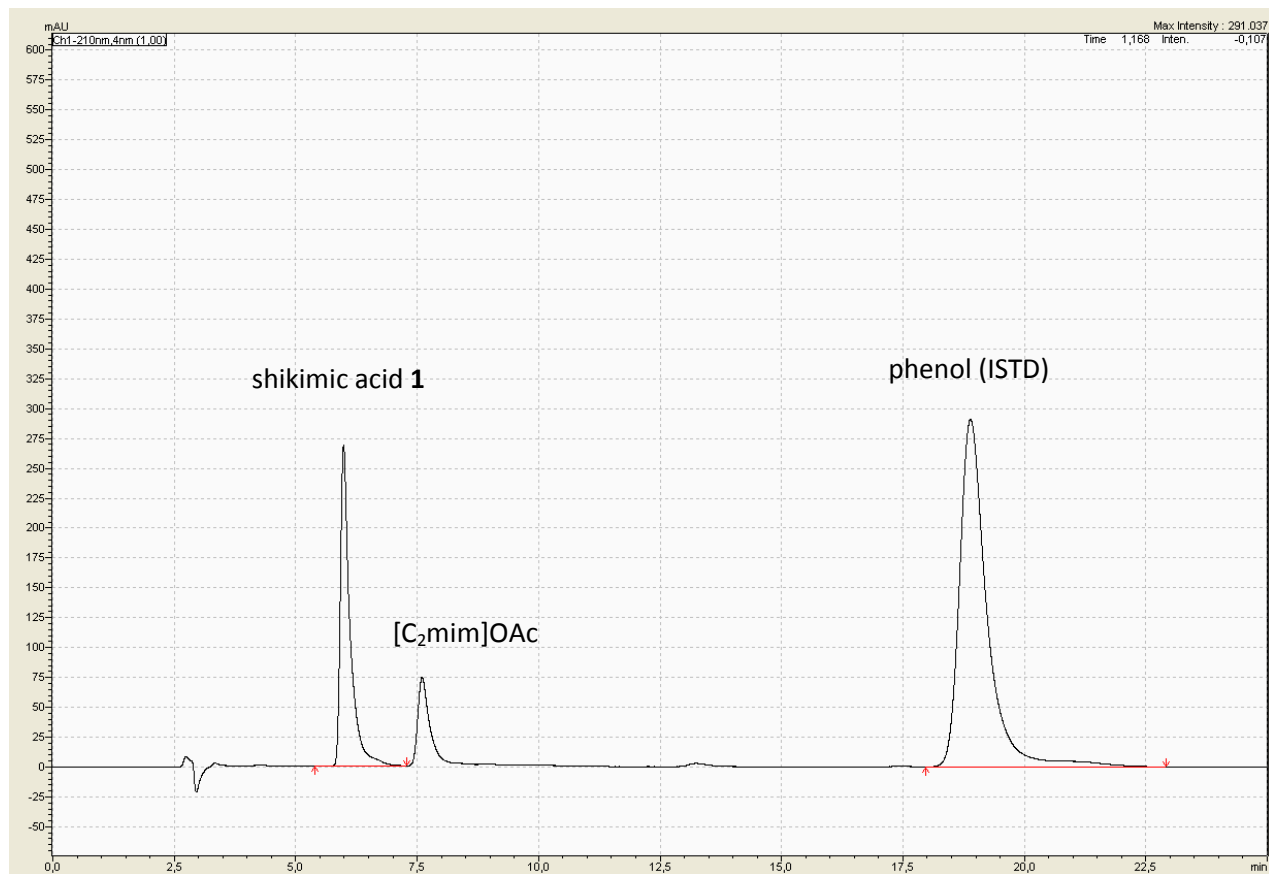
^b *Institute of Applied Synthetic Chemistry, Vienna University of Technology, 1060 Vienna, Austria; Fax: +43 1 58801 16360; Tel: +43 1 58801 163601; Email: kbica@ioc.tuwien.ac.at*

^c *Institute of Computational Biological Chemistry, University of Vienna, Austria; Tel: +43 1 4277 52711; E-mail: christian.schroeder@univie.ac.at*

1. Fig. S1: Calibration curve for the determination of shikimic acid 1 using phenol as internal standard



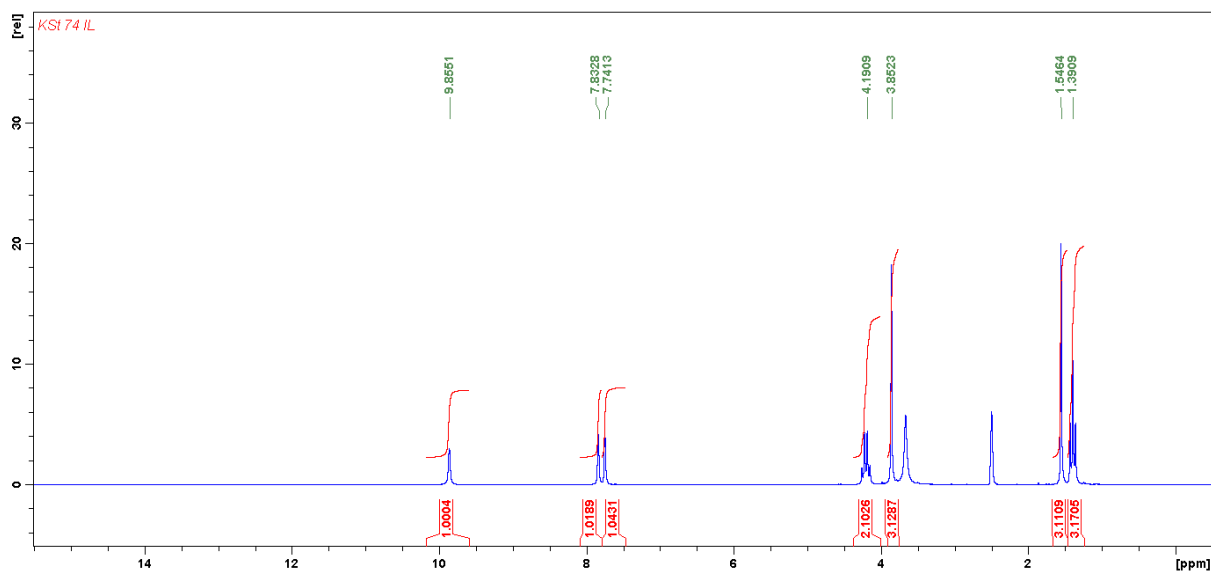
2. Fig. S2: Representing chromatogram for the determination of shikimic acid in the presence of ionic liquid



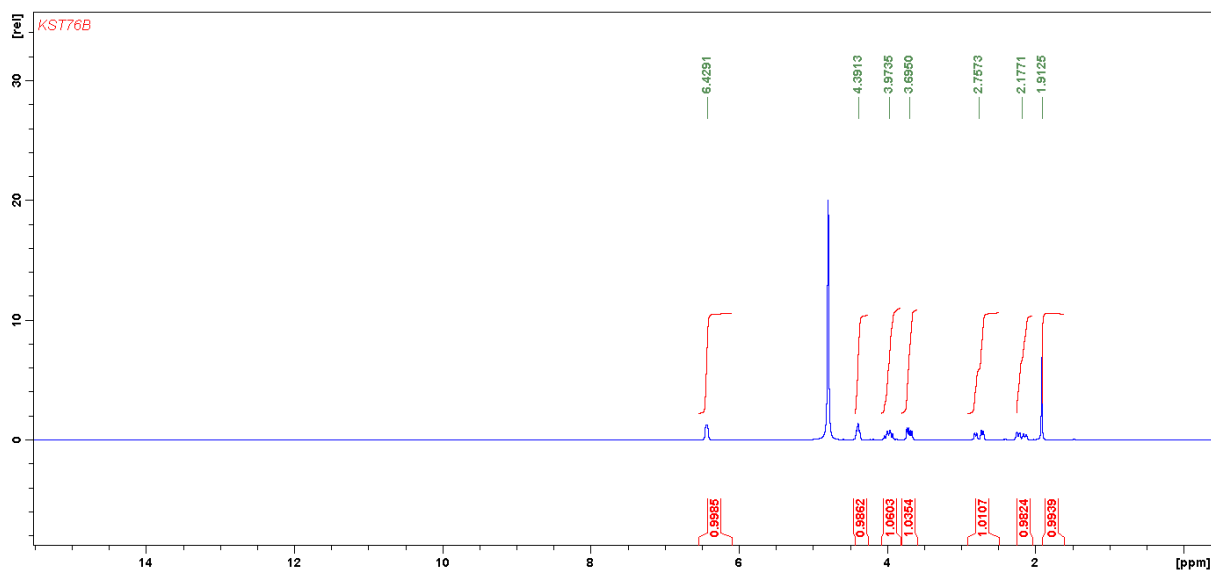
10 wt.% star anise powder in [C₂mim]OAc; rt, 24 h

Phenomenex Resex RHM-monosaccharide H⁺ column (150 × 7.80 mm), H₂O/5% TFA, 0.6 ml/min, detection 210 nm

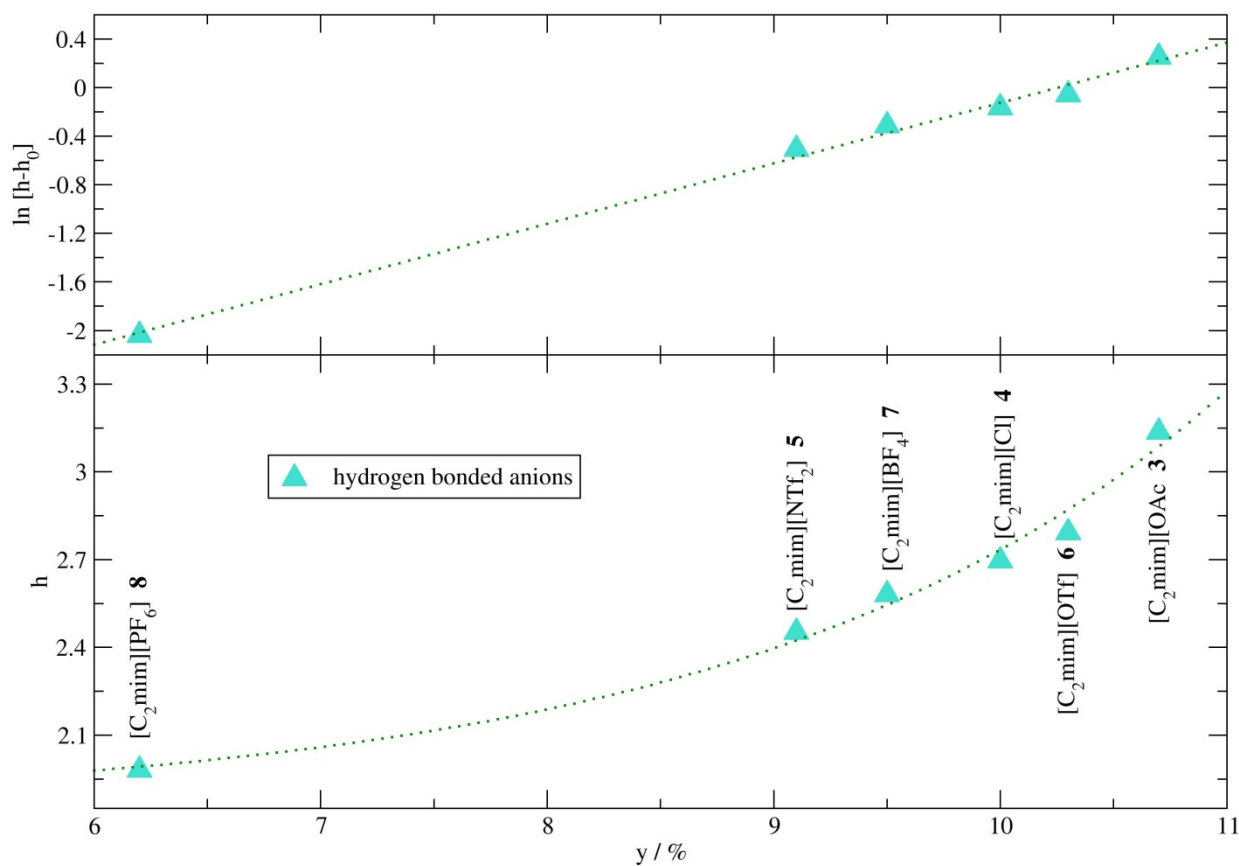
3. Fig. S3: ^1H NMR spectra of recovered ionic liquid 1-ethyl-3-methylimidazolium acetate
[C₂mim]OAc



4. Fig. S4: ^1H NMR spectra of isolated shikimic acid



5. Fig. S5: Correlation between the extraction yield and the number of hydrogen bonded anions



The number of hydrogen bonded anions h seems to depend exponentially on the extraction yield y

$$h = h_0 + A e^{a \cdot y}$$

with $h_0 = 1.85$, $A = 0.00609$ and $a = 0.4976$. The subfigure on top represents a corresponding linear-log plot. Here, the exponential behavior can be determined by a linear regression with $R^2 = 0.9945$.