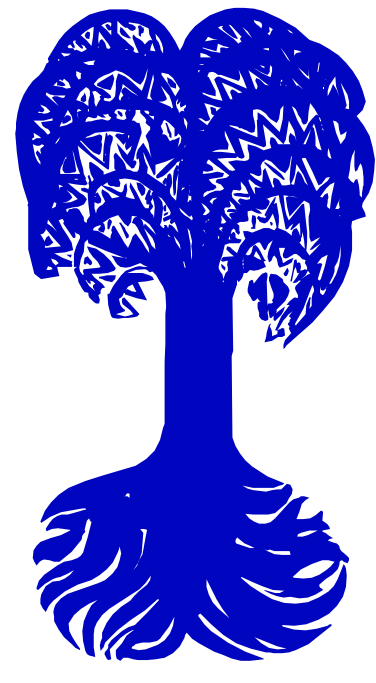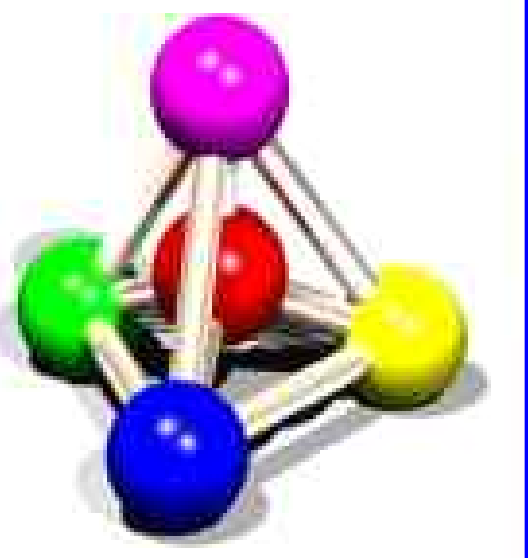# Parallel Detection of R22 and its Substitutes by Reflectometric Interference Spectroscopy

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Introduction

- Chlorofluorocarbons like R22 are known to destroy the ozone layer.

- Substitutes still have an enormous global warming potential, therefore a recycling process is highly desirable.

- A fast and reliable classification and quantification of returned substances is of interest, as they are often contaminated by chlorofluorocarbons.

- The microporous polycarbonate Makrolon® (mean pore size volume: 0.1 nm³) was used as sensitive layer: discrimination of the analytes by utilitzing a molecular sieve effect.

Principle of RIfS

- **Conduction principle: Reflectometric Interference Spectroscopy, using a single-sensor setup.**
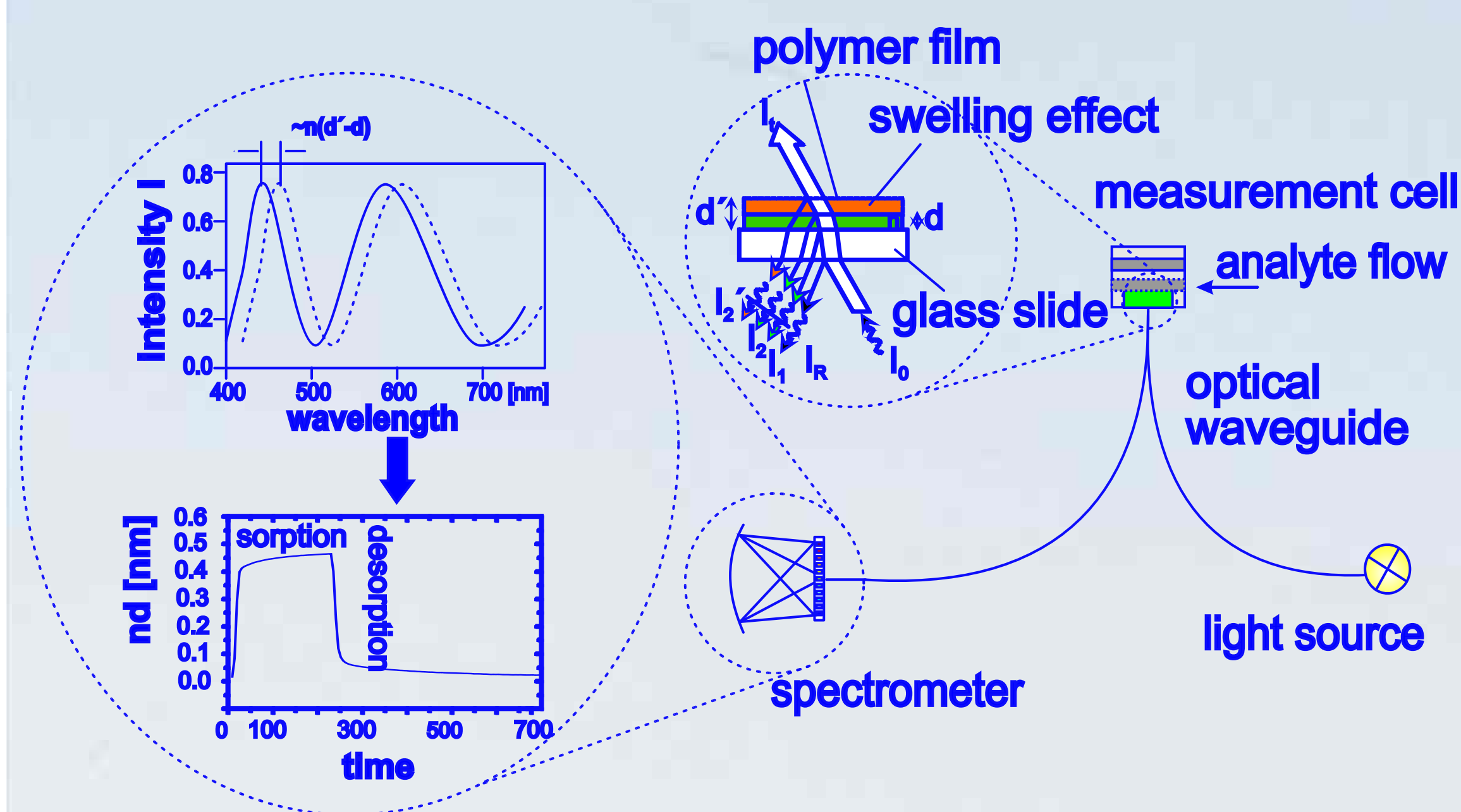
- Reflection of white light at thin layer interfaces results in typical interference pattern.

- Reversible swelling of the sensitive polymer layer due to analyte exposition causes a change in optical thickness.

- Change of the position of extremum is evaluated.

Response Signals of the Analytes
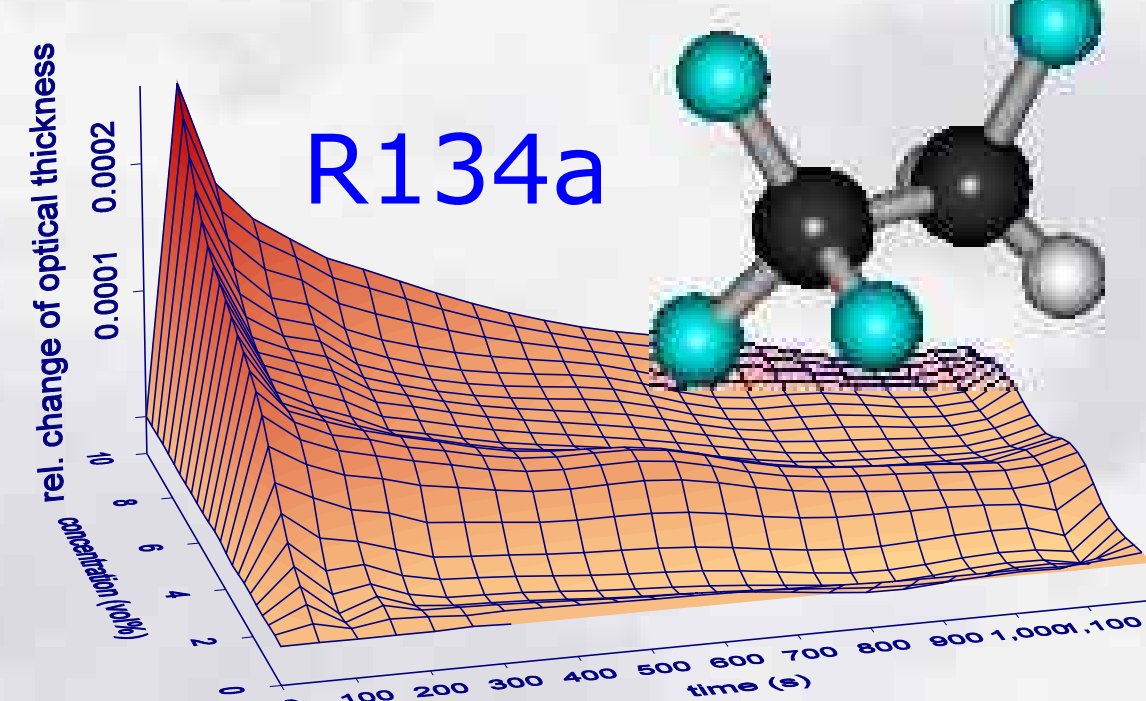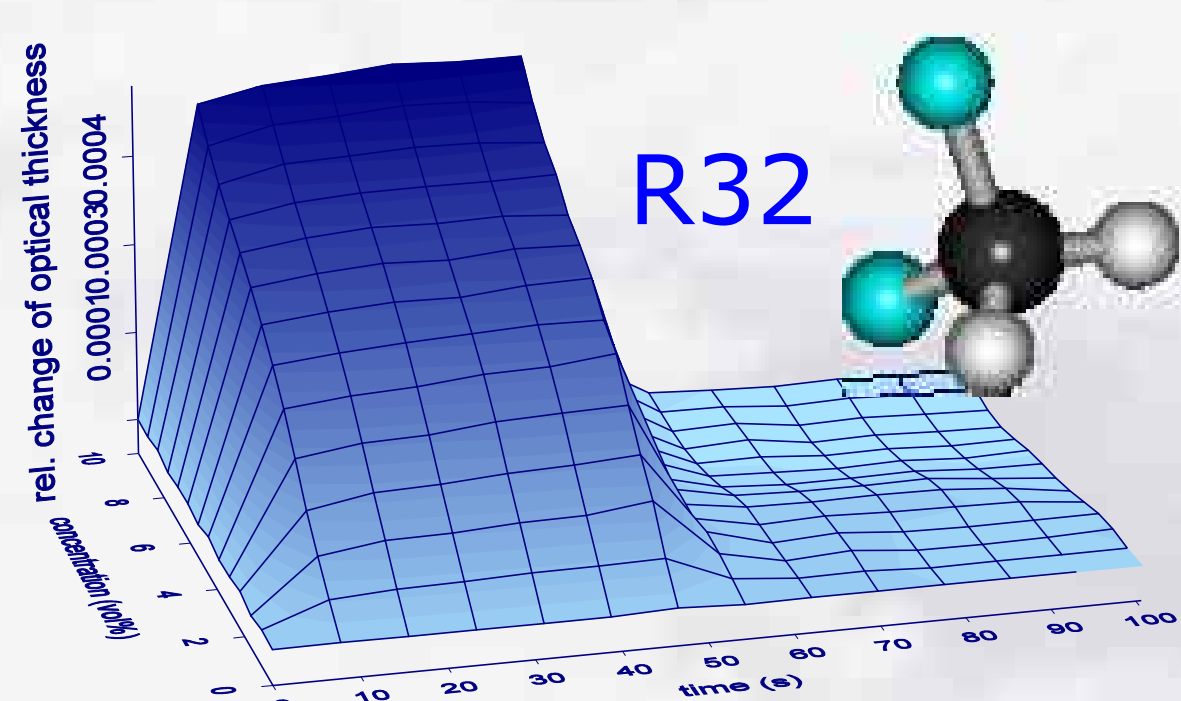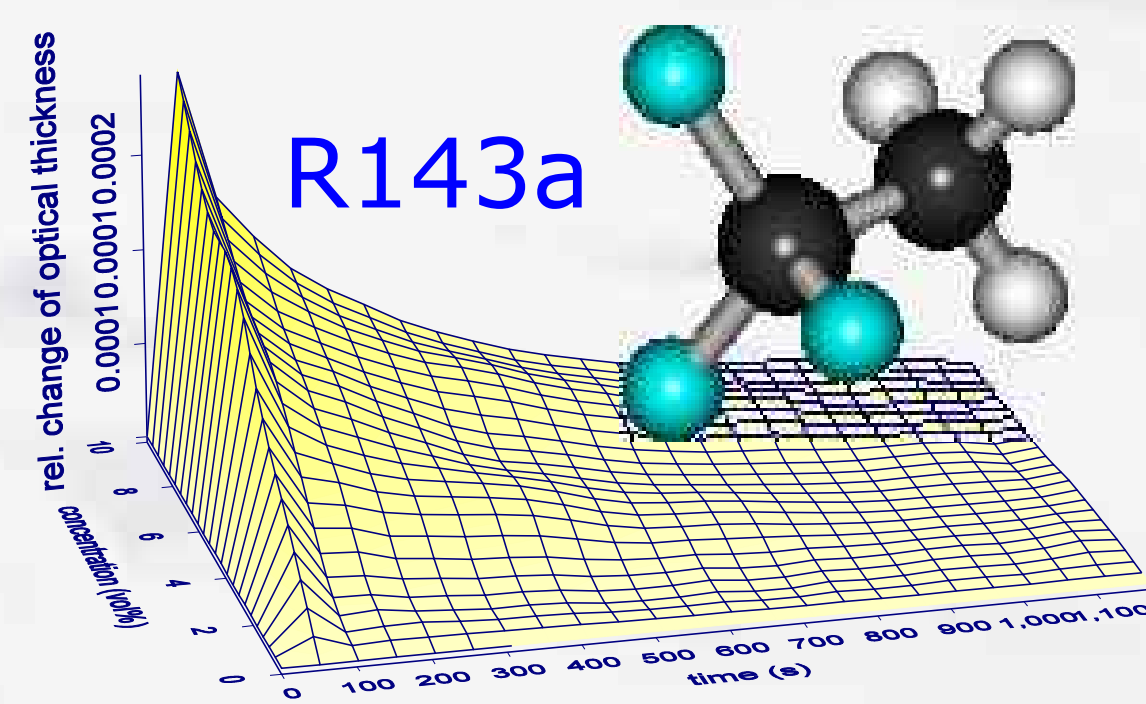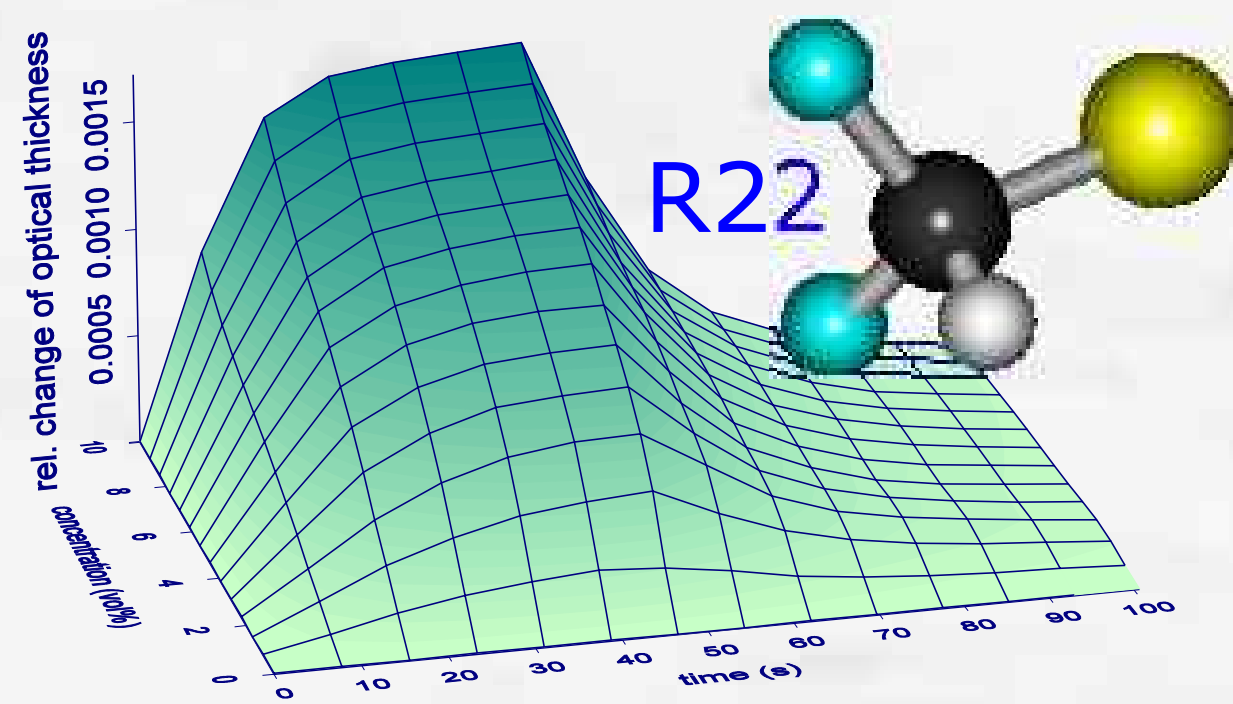
- small analytes show fast sorption and desorption kinetics

- longer regeneration period required for the bigger analytes

- Different sensor responses in shape as well as in hight for all analytes at all time-points.

- Sensor responses at different times can be used as "virtual sensors" to minimize the number of sensitive layers when evaluated by neural networks.

- Only one "real" sensor for up to 4 analytes.

Measurements and Data Evalution

- Two different full-factorial designs of ternary mixtures of R22 and its substitutes were measured.

- Calibration data (for training): 6-level equidistant design with concentrations of 0 - 10 vol%: 216 different mixtures.

- Validation data (independent test data): 5-level equidistant design with a concentration range of 1 - 9 vol%: 115 different mixtures.

- One neural network for each analyte.

- Optimisation of evaluation: feature selection for growing neural networks with up to 15 input neurons for each net.

Results
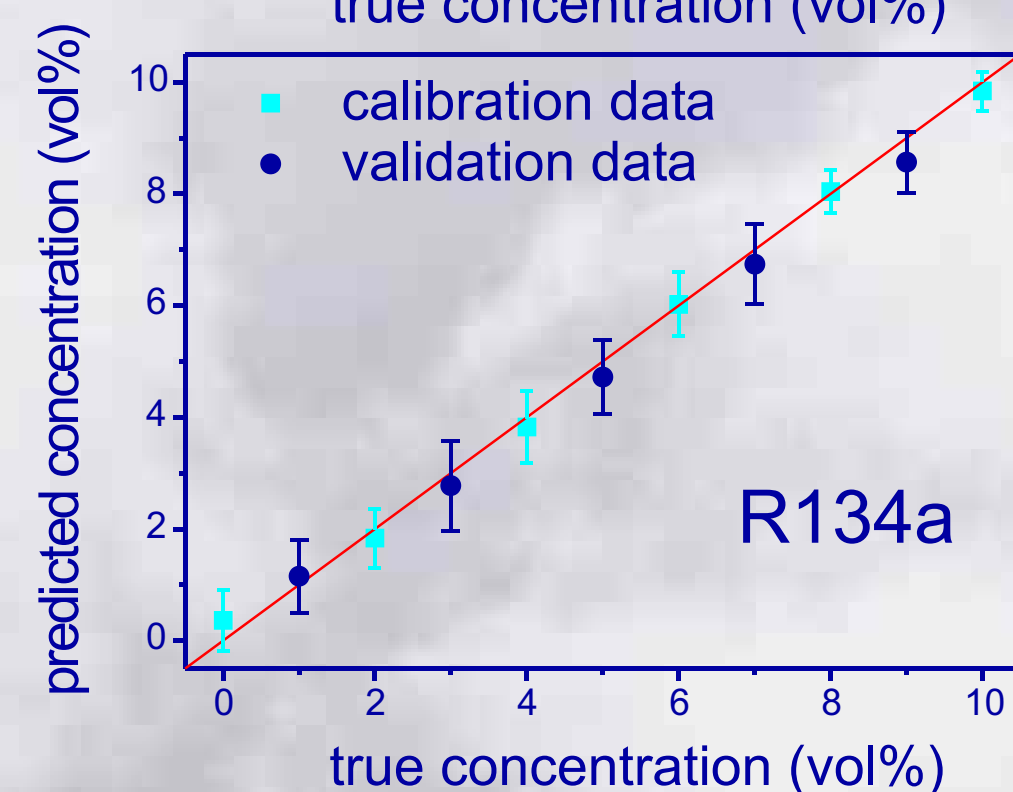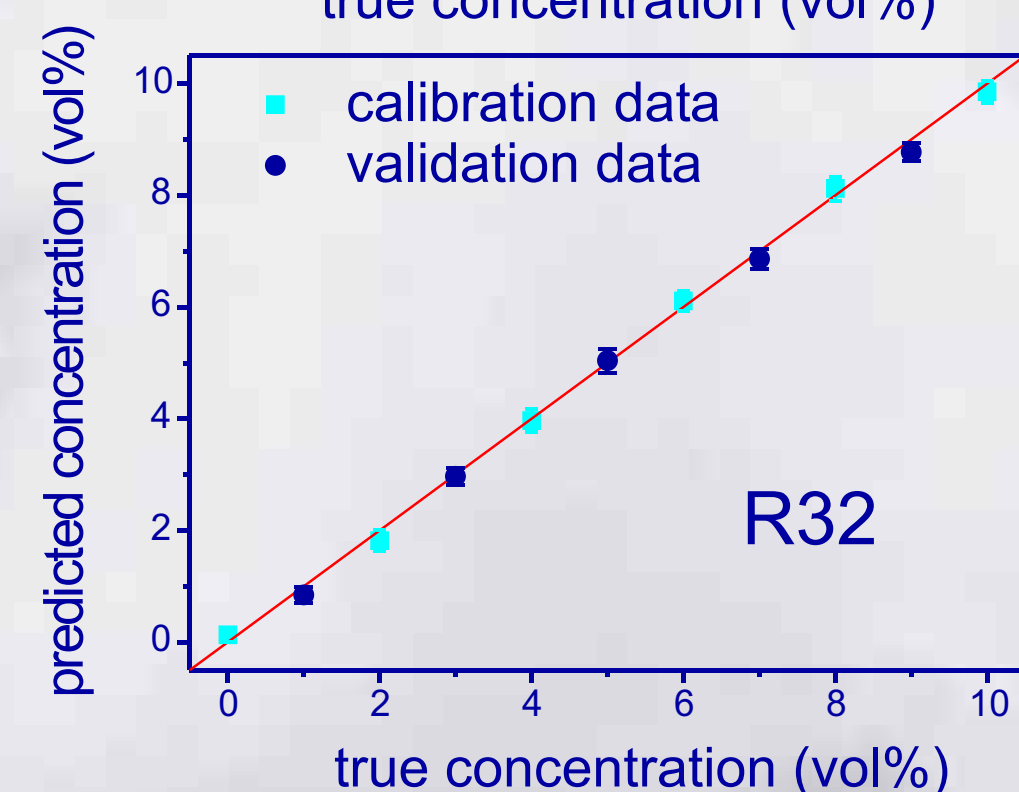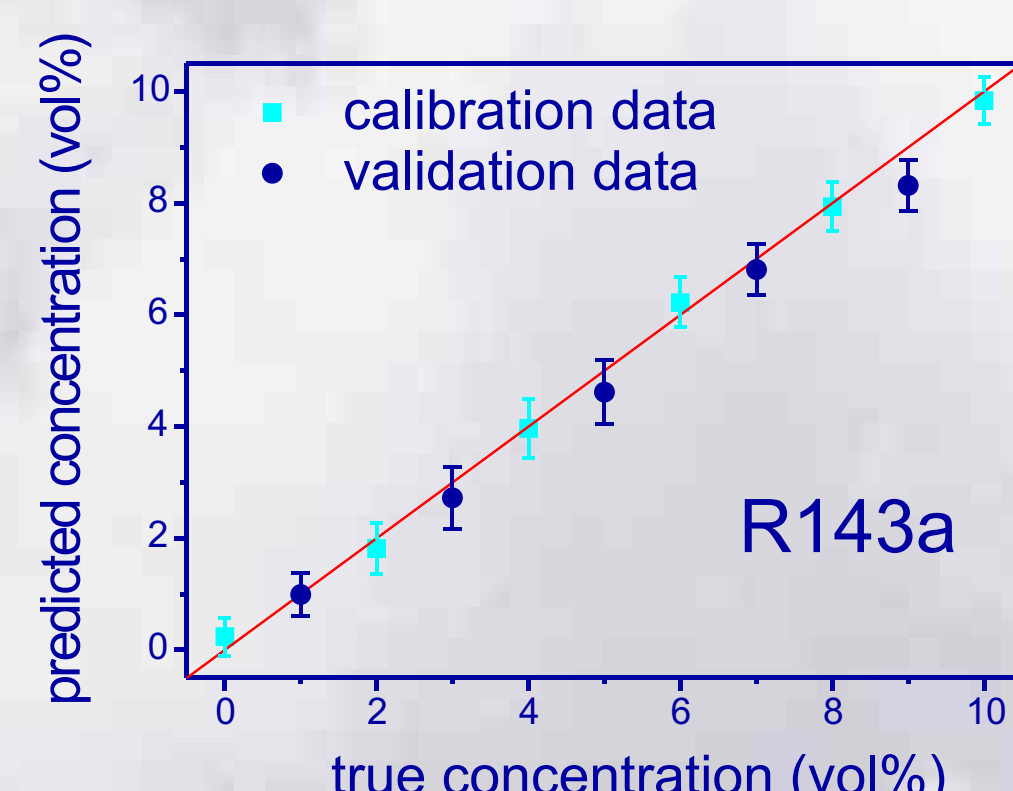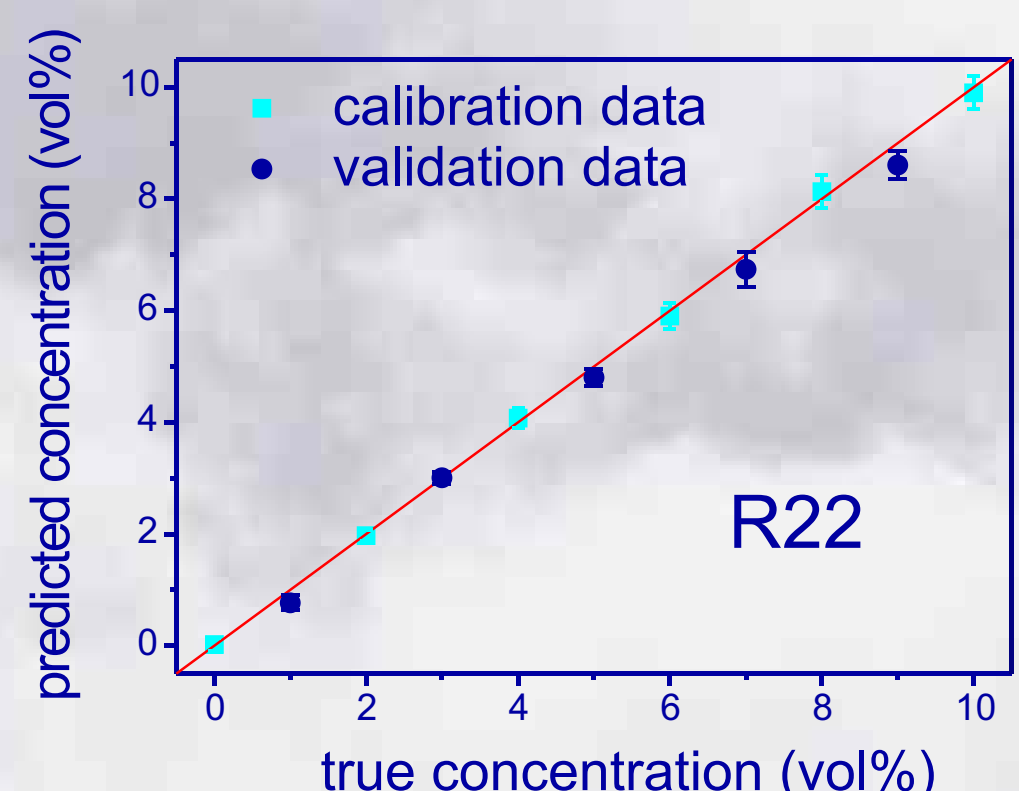
- The true-predicted plots show that the predictions of all analytes are unbiased: the means of all concentration levels do not deviate significantly from the diagonal.

- Smaller standard deviations for the smaller analytes.

RSME (%)	calibration data	validation data
R22	4.58	6.48
R32	4.52	4.33
R134a	9.31	12.28
R143a	10.89	14.53

Summary

- All analytes can be determined quantitatively in ternary mixtures by a single sensor RIfS setup.

Outlook

- Measurements of ternary mixtures with our low-cost RIfS setup.

- Measurements of quaternary mixtures with a sensor array using microporous polymers with various mean pore size volumes.

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