

# Tests of suitable vials and caps for PFAS (per- and polyfluoroalkyl substances) analysis

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## Abstract

This note describes the evaluation of different vials and caps for per- and polyfluoroalkyl substances (PFAS) analysis. It investigates suitability of silanized glass vials and various plastic vials by determining the adsorption effect through signal strength measurements. Additionally it contains tests on possible contaminants from the sampling unit.

## Introduction

Per- and polyfluoroalkyl substances (PFAS) are a group of persistent and bioaccumulative anthropogenic pollutants characterized by a linear aliphatic backbone, a high degree of fluorination and often feature a carboxylic or sulfonic acid functionality. PFAS are common to consumer and industrial processes around the globe. They are introduced to the environment through a variety of sources such as food contact materials, manufacturing or industrial applications. Because of the accumulation of PFAS in water, soil and living organisms and the well-known health risks associated with PFAS exposure it is important to ensure proper worldwide monitoring of these chemicals.

## Test conditions

- Standard solutions are tested and compared in different vials
- Concentration 2 ng/mL
- Solvent composition (Water %/Methanol %): 60/40; 50/50; 40/60
- Number of samples: BL n = 1, P n = 3
- The samples are stored and analysed repeatedly on different days
  - Series triple injection
  - Series after 24 hours triple injection

## Products under evaluation

- 702079: Silanized screw neck vial N 9, 11.6x32.0 mm, 1.5 mL, label + filling lines, flat bottom, amber
- 702010: Polypropylene screw neck vial N 9, 11.6x32.0 mm, 0.7 mL, with round bottom insert, transparent (702009 with 0.3 mL was not tested, as design and material wise identical to 702010)
- 702500: Polypropylene screw neck vial N 9, 11.6x32.0 mm, 1.5 mL, flat bottom, transparent, filling lines
- 702402: PP screw cap N 9, blue, center hole, Silicone white/ Polyimide orange, 1.0 mm, fluorine-free

## Evaluation basis for measuring the adsorption effects

- Samples with 40 % – 60 % relative proportion of methanol in the sample solution are considered, since only in this area both short and long-chain PFAS dissolve satisfactorily in the sample vials.
- As reference point a measuring point with optimal relative signal strength is fixed and all measurement data from the test series are compared to that.
- Evaluation of the data from both the first injection and the repeated injection after 24 hours.

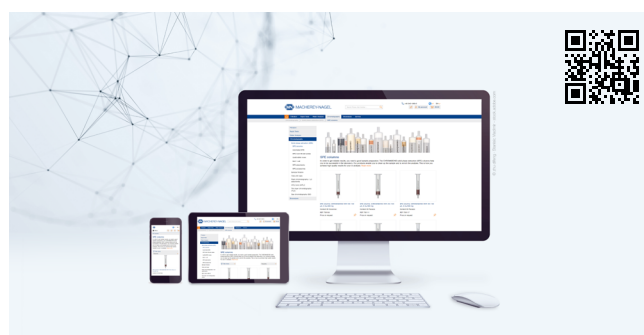
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# Suitable vials and caps for PFAS analysis

Measurement of the relative signal intensity (%) compared to the measuring point with optimal relative signal strength

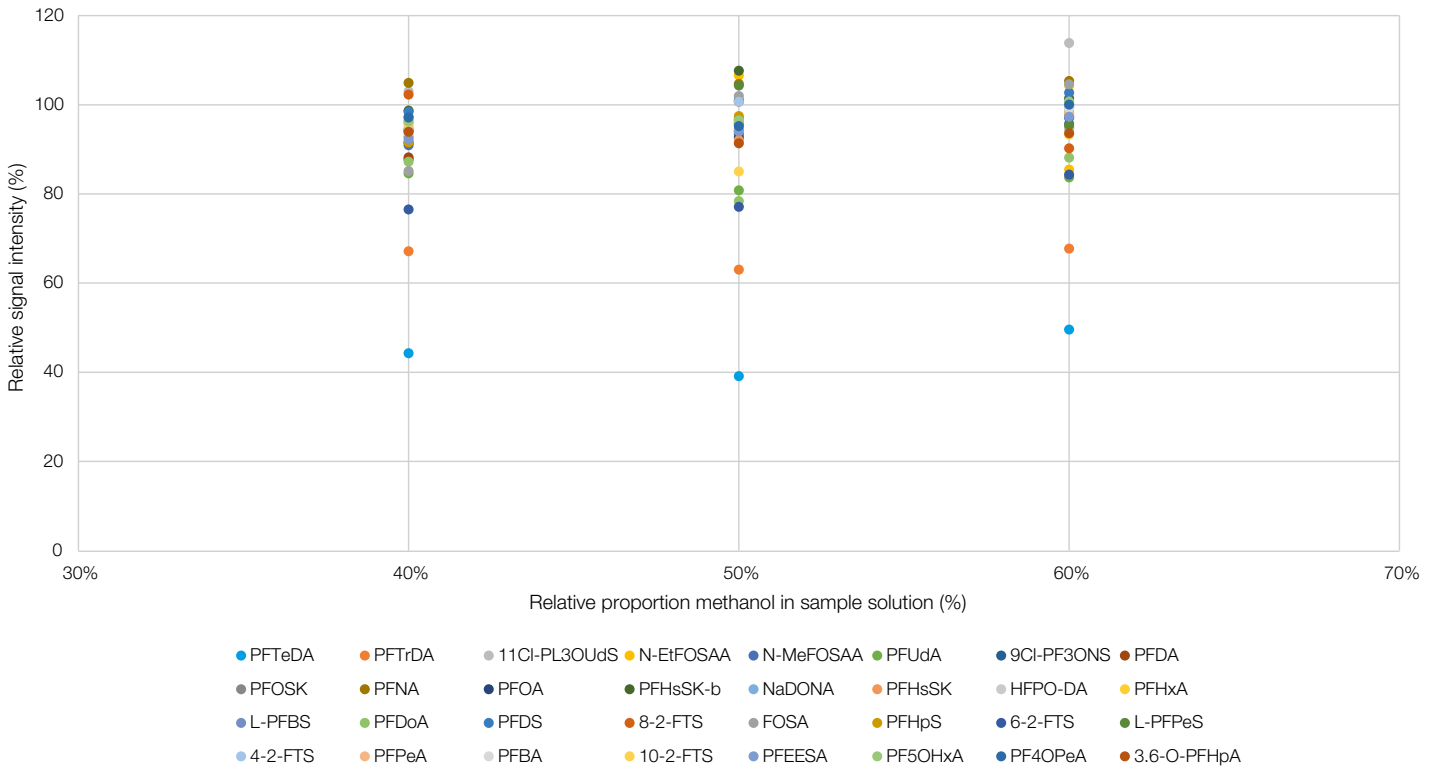


Figure 1: REF 702079 Silanized screw neck vial N 9, 11.6x32.0 mm, 1.5 mL, label + filling lines, flat bottom, amber with REF 702402 PP screw cap N 9, blue, center hole, Silicone white/Polyimide orange, 1.0 mm, fluorine-free

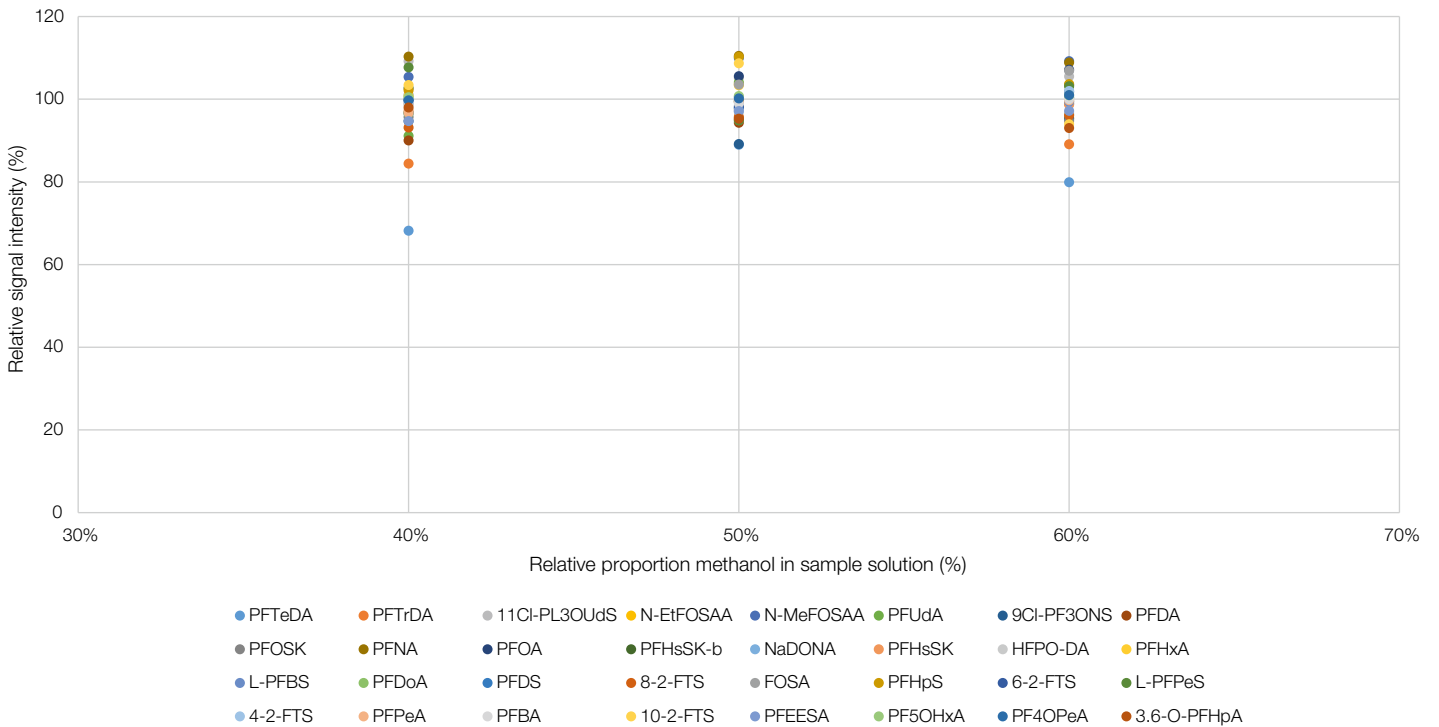


Figure 2: REF 702010 Polypropylene screw neck vial N 9, 11.6x32.0 mm, 0.7 mL, with round bottom insert, transparent with REF 702402 PP screw cap N 9, blue, center hole, Silicone white/Polyimide orange, 1.0 mm, fluorine-free

## Suitable vials and caps for PFAS analysis

Measurement of the relative signal intensity (%) compared to the measuring point with optimal relative signal strength

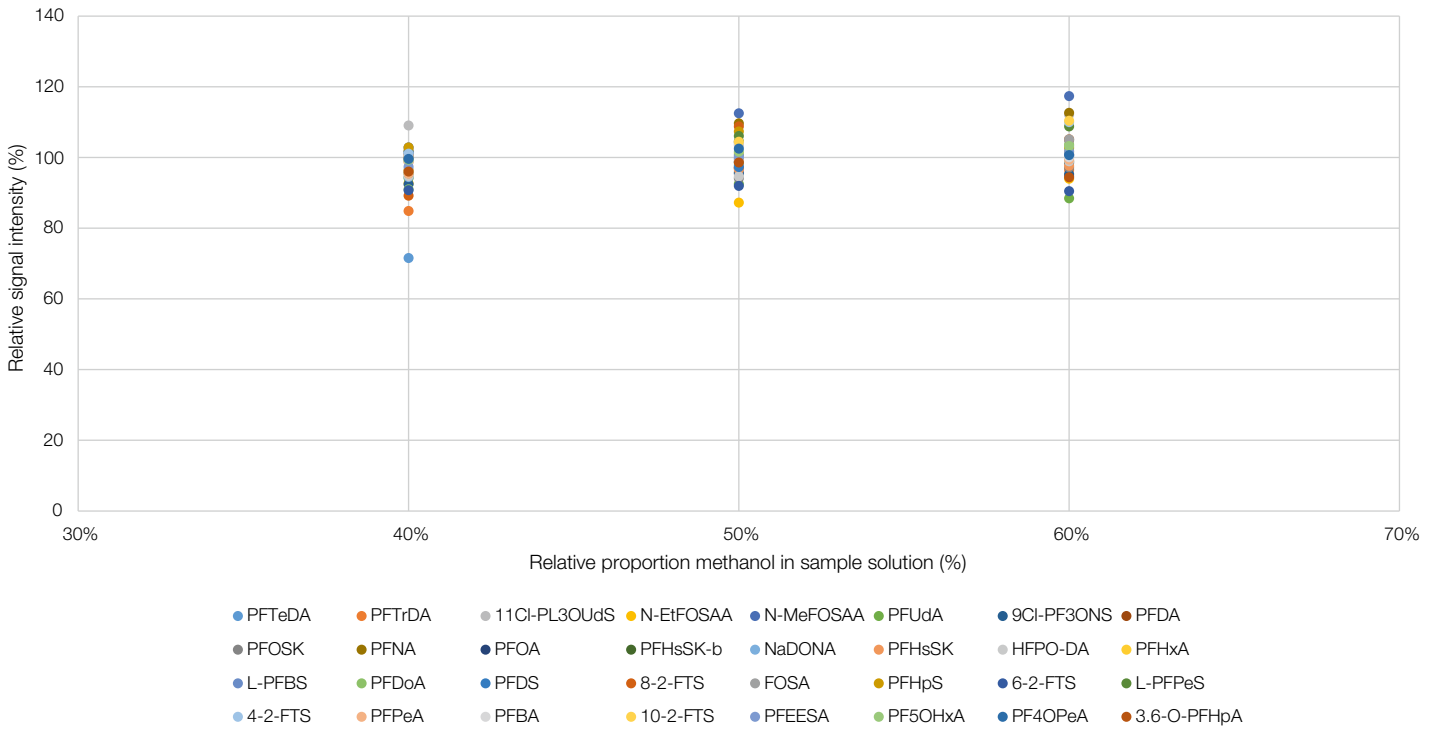


Figure 3: REF 702500 Polypropylene screw neck vial N 9, 11.6 x 32.0 mm, 1.5 mL, flat bottom, transparent, filling lines with REF 702402 PP screw cap N 9, blue, center hole, Silicone white/Polyimide orange, 1.0 mm, fluorine-free

Even after 24 hours the results with regard to the signal intensity of both PP vials are still considerably better than that of the silanized glass vial.



Figure 4: MACHEREY-NAGEL Polypropylene vials and fluorine-free closures for PFAS analysis

# Suitable vials and caps for PFAS analysis

## Measurement of the relative average intensity (%)

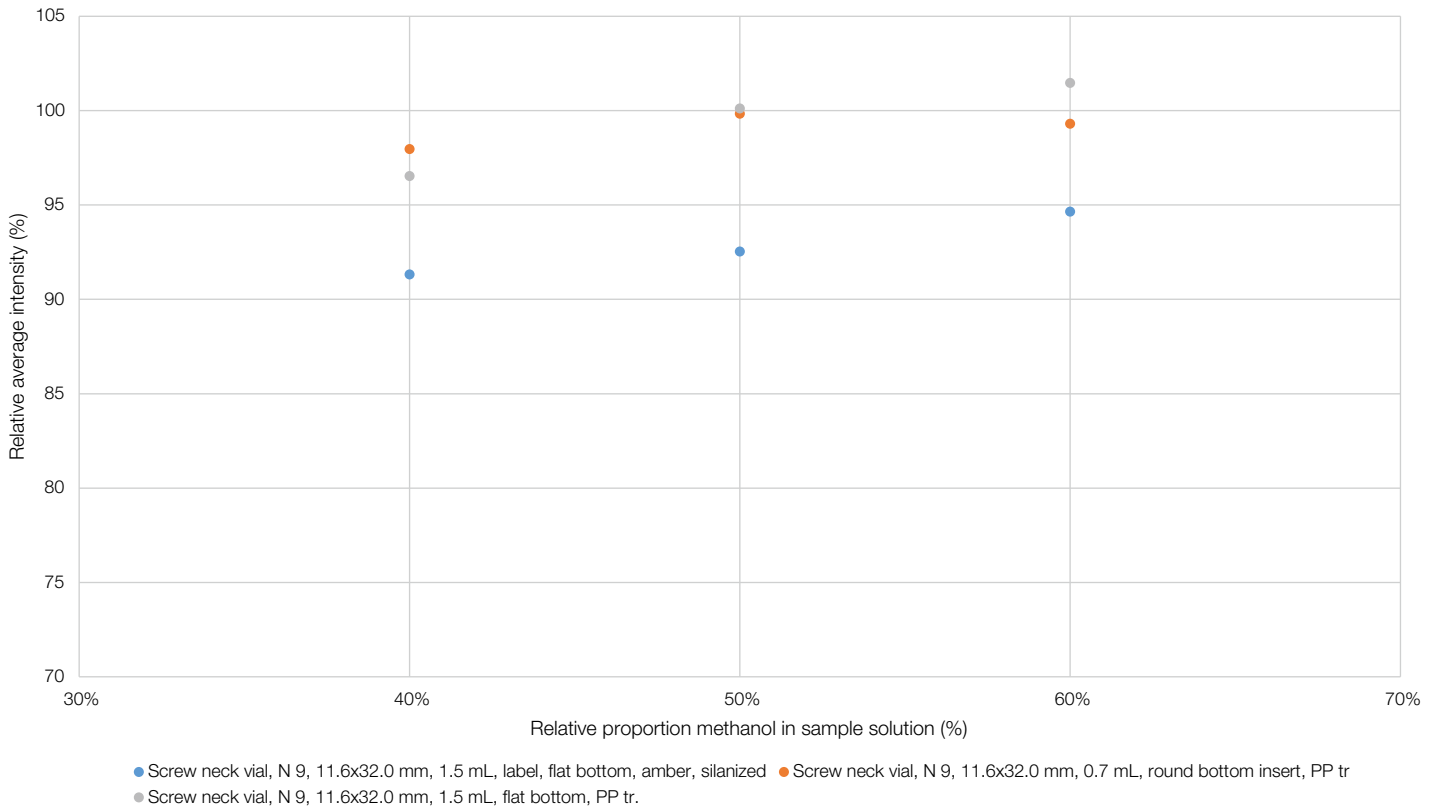


Figure 5: Relative average intensity (%), Standard solution 2 ng/mL

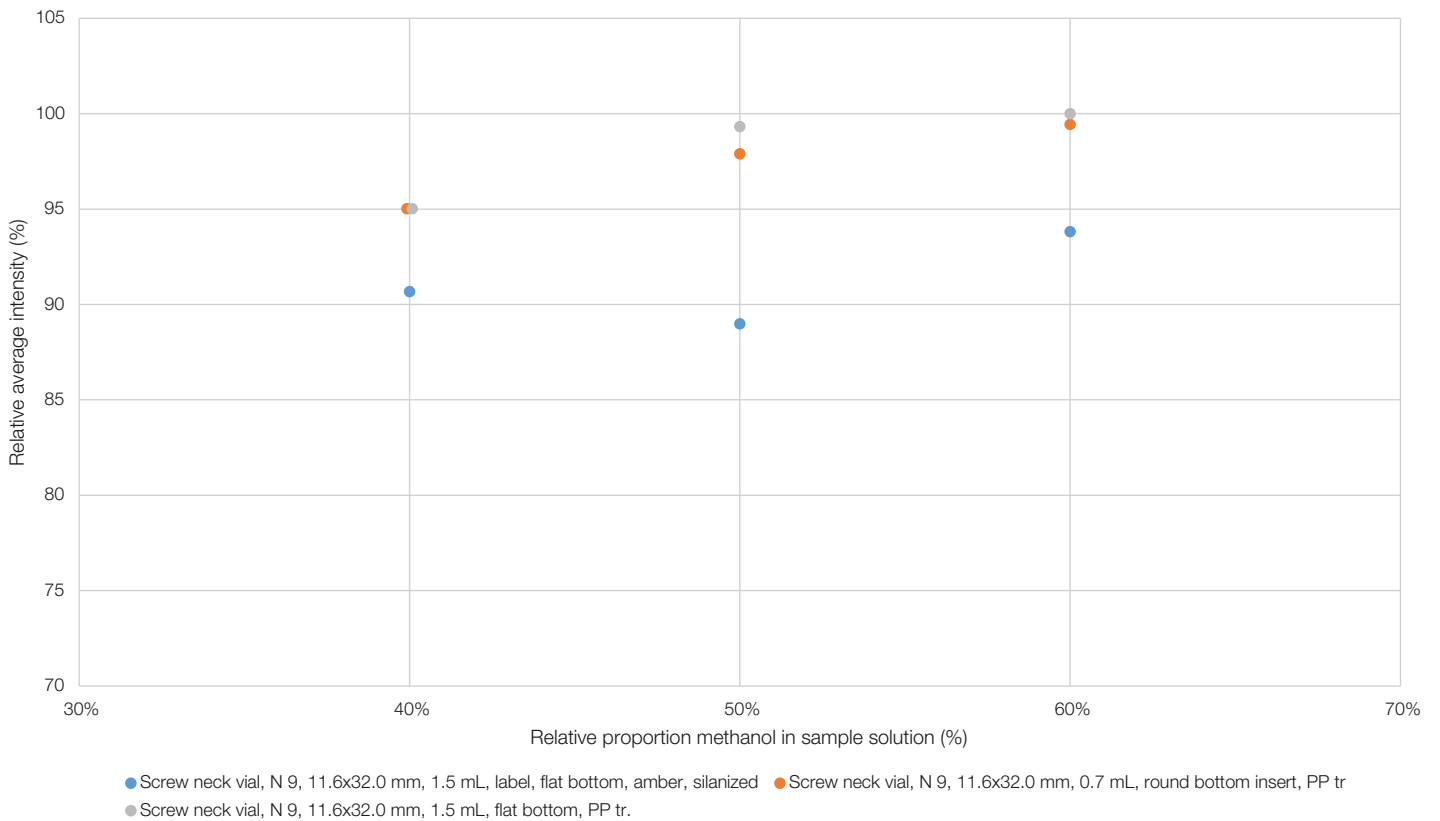


Figure 6: Relative average intensity (%), Standard solution 2 ng/mL; repeated measurement after 24 hours

# Suitable vials and caps for PFAS analysis

## Measurement of the number of PFAS below 95 % of the max. signal intensity (%)

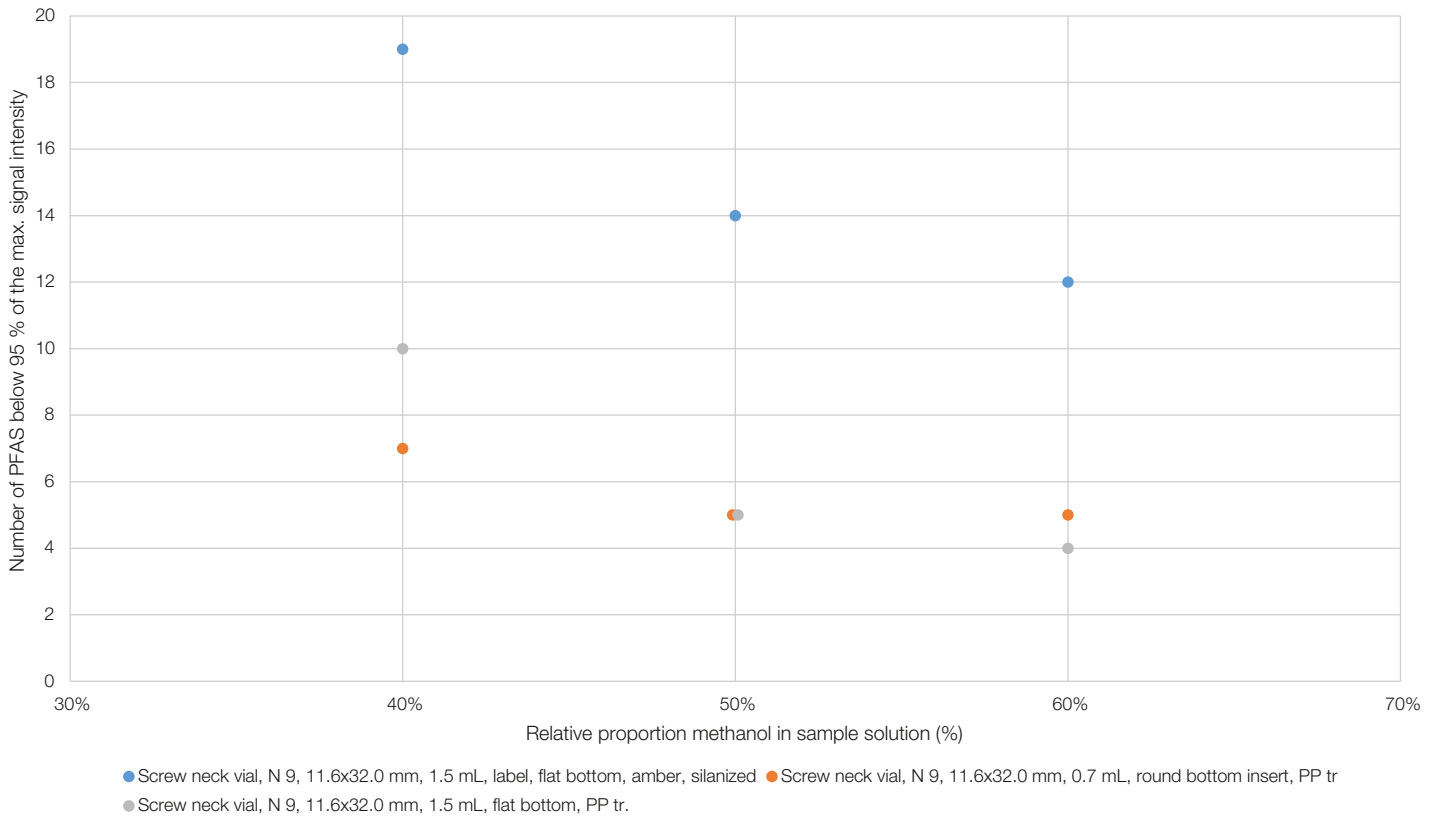


Figure 7: Number of PFAS below 95 % of the max. signal intensity, Standard solution 2 ng/mL

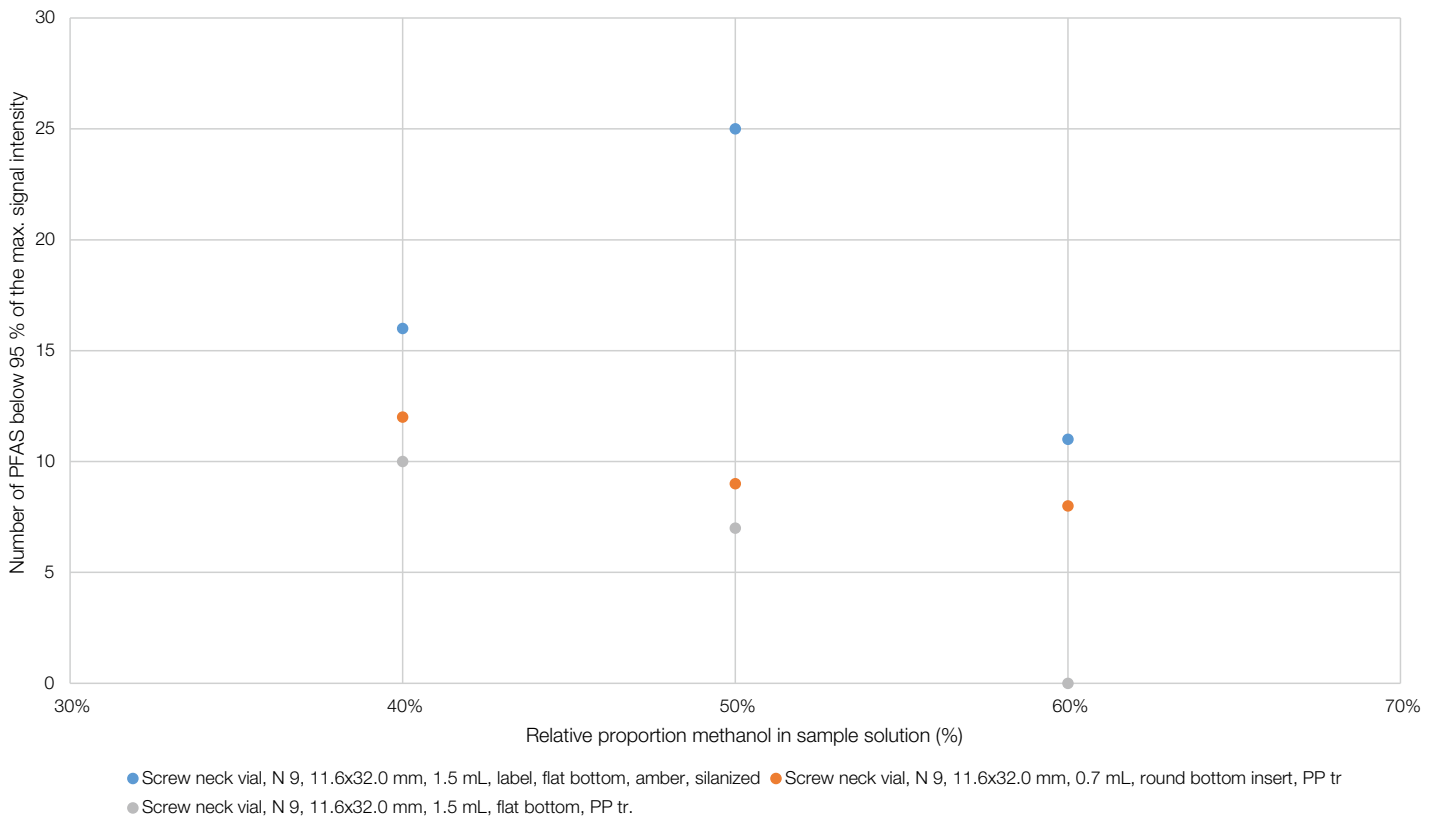


Figure 8: Number of PFAS below 95 % of the max. signal intensity, Standard solution 2 ng/mL; repeated measurement after 24 hours

# Suitable vials and caps for PFAS analysis

## Test results

- Despite silanization the glass walls show significant adsorption effects
- The number of PFAS with these effects is significantly larger with glass
- Both PP vial types are equivalent
- Long-chain Perfluoroalkylcarboxylic Acids are particularly affected
- Ghostpeaks by contaminants:  
Only with PFBA (Perfluorobutanesulfonic acid) ghostpeaks below 1 % could be seen (especially when the aqueous proportion was larger). This could be related to the polarity of the analyte or to a higher pollution of the ultrapure water. Exemplary below PFBA (Perfluorobutanesulfonic acid)

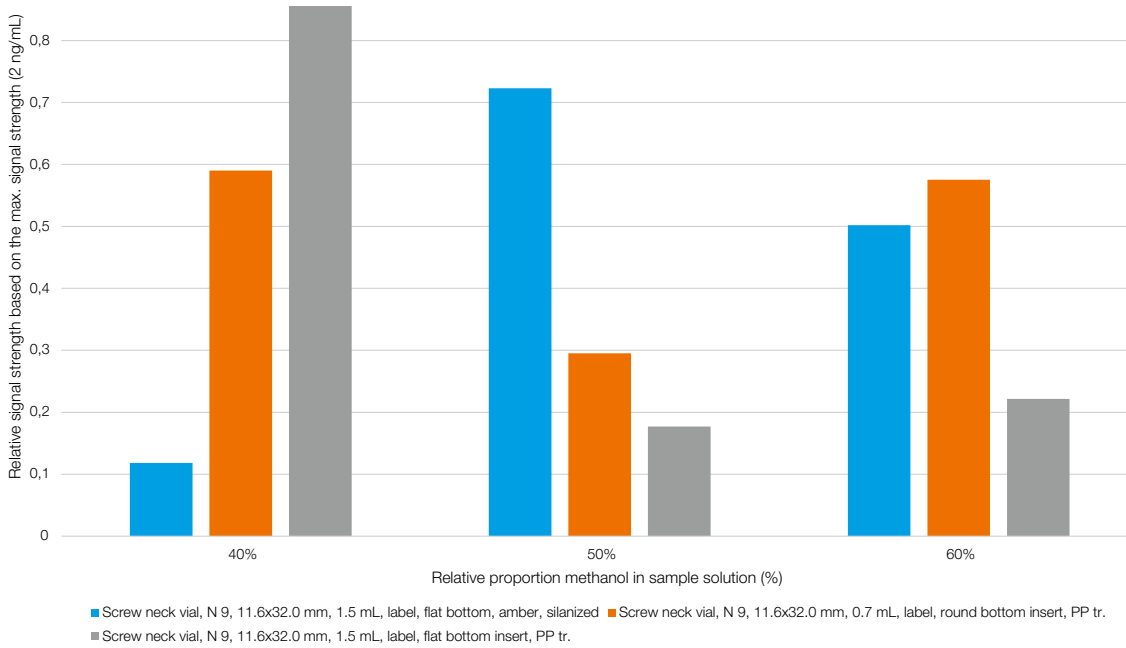


Figure 9: Perfluorobutanesulfonic acid (PFBA) ghostpeaks

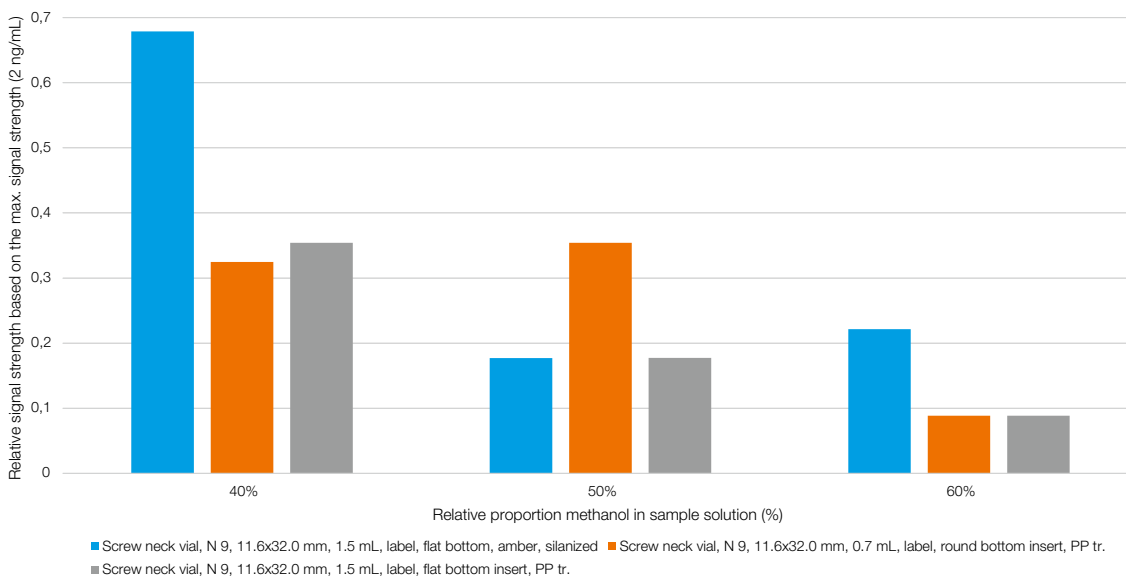


Figure 10: Perfluorobutanesulfonic acid (PFBA) ghostpeaks; comparison after 24 hours

## Suitable vials and caps for PFAS analysis

### Conclusion

Polypropylene vials are the best choice for doing PFAS analysis, as the adsorption effect is the lowest and thus the signal strength of the analytes the best. Contaminations either from the plastic of the vial or from the septa material are neglectable, as even with PFBA below 1 %.

Fluorine-free septa, i. e. septa with a Polyimide instead of a PTFE lamination, are recommendable to exclude any migration of fluorine into the sample.

### Product information

The following MACHEREY-NAGEL products are related to this test note:

- REF 702009 Polypropylene screw neck vial N 9, 11.6 x 32.0 mm, 0.3 mL, with inner cone, transparent
- REF 702172 Polypropylene screw neck vial N 9, 11.6 x 32.0 mm, 0.3 mL, with inner cone, amber
- REF 702010 Polypropylene screw neck vial N 9, 11.6 x 32.0 mm, 0.7 mL, with round bottom insert, transparent
- REF 702500 Polypropylene screw neck vial N 9, 11.6 x 32.0 mm, 1.5 mL, flat bottom, transparent, filling lines
- REF 702402 PP Screw closure N 9. blue, center hole, Silicone. white/Polyimide orange, 1.0 mm, fluorine-free
- REF 702809 Polypropylene snap ring vial N 11, 11.6 x 32.0 mm, 0.3 mL, with inner cone, transparent
- REF 702173 Polypropylene snap ring vial N 11, 11.6 x 32.0 mm, 0.3 mL, with inner cone, amber
- REF 702174 Polypropylene snap ring vial N 11, 11.6 x 32.0 mm, 0.7 mL, with round bottom insert, transparent
- REF 702403 PE Snap ring closure N 11. soft, bright blue, center hole, Silicone. white/Polyimide orange, 1.0 mm, fluorine-free
- REF 702819 Polypropylene micro-insert for wide opening, 5.7 x 29 mm, 0.1 mL, transparent, with spring

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