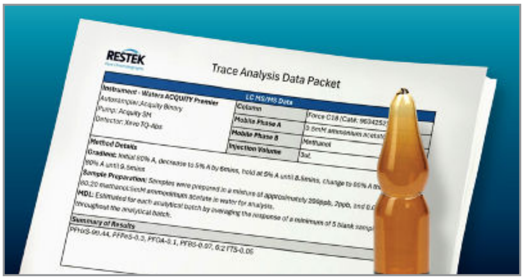
How to Read a Trace Analysis Data Packet

Trace analysis data packets, which are part of our expanded data packs for Restek's single and multicomponent PFAS reference standards, include detailed information to help you understand the composition of your standards. This article explains how to read your packet, using our br-PFHxS standard (cat.# 30803) as an example.

> *You can access the trace analysis data packet for your standard by using our documentation search tool (restek.com/documentation) and entering your standard's cat.# and lot #. You can also access your standard's certificate of analysis (CofA) at the same location.*



Restek's trace analysis data packets include data from two methods, each for a different purpose. The first section of the data pack uses LC-MS/MS for trace analysis of samples. The second section, which is explained later in this article, uses NMR to identify individual isomers.

LC-MS/MS Trace Analysis of Samples

Analytical Method Summary Table

The first table (figure 1) within the trace analysis data packet includes a summary of the analytical method used for trace analysis of samples.

Figure 1: LC MS/MS Data

<table>
<tr><th colspan="3">LC MS/MS Data</th></tr>
<tr><td rowspan="4">Instrument - Waters ACQUITY Premier
Autosampler: Acquity Binary
Pump: Acquity SM
Detector: Xevo TQ-Abs</td><td>Column</td><td>Force C18 (Cat#: 9634252)</td></tr>
<tr><td>Mobile Phase A</td><td>0.5mM ammonium acetate in water</td></tr>
<tr><td>Mobile Phase B</td><td>Methanol</td></tr>
<tr><td>Injection Volume</td><td>3uL</td></tr>
<tr><td colspan="3">Method Details
Gradient: Initial 80% A, decrease to 5% A by 6mins, hold at 5% A until 8.5mins, change to 80% A then hold at 80% A until 9.5mins
Sample Preparation: Samples were prepared in a mixture of approximately 200ppb, 2ppb, and 0.02ppb in 80:20 methanol:5mM ammonimum acetate in water for analysis.
MDL: Estimated for each analytical batch by averaging the response of a minimum of 5 blank samples run throughout the analytical batch.</td></tr>
<tr><td colspan="3">Summary of Results</td></tr>
<tr><td colspan="3">PFHxS-99.44, PFPeS-0.3, PFOA-0.1, PFBS-0.07, 6:2 FTS-0.05</td></tr>
</table>

Method detection limit (MDL) is determined in each analytical batch to ensure there is no background contamination within the instrument. This is used to determine the final LOQ.

The **Summary of Results** for each analyte is measured >LOQ in % wt.

MRM Transitions Table

The second table (figure 2) contains an analyte list and transitions measured by the trace analysis.

Figure 2: MRM Transitions

Compound	Parent Ion 1	Daughter Ion 1	Parent Ion 2	Daughter Ion 2
PFBA	213	169		
PFMPA	229	85		
3:3FTCA	241	117	241	177
PFPeA	263	69	263	219
PFMBA	279	85		
HFPO-DA	285	169	285	185
NFDHA	295	85	295	201
PFBS	299	80	299	99
PFHxA	313	119	313	269
PFEESA	315	83	315	135
4:2 FTS	327	81	327	307
5:3FTCA	341	217	341	237
PFPeS	349	80	349	99
PFHpA	363	169	363	319
ADONA	377	85	377	251
PFHxS	399	80	399	99
PFOA	413	169	413	369
6:2 FTS	427	81	427	407
7:3 FTCA	441	317	441	337
PFHpS	449	80	449	99

Compound	Parent Ion 1	Daughter Ion 1	Parent Ion 2	Daughter Ion 2
PFNA	463	219	463	419
PFOS	499	80	499	99
FOSA	498	78	498	478
NMeFOSA	512	169	512	219
PFDA	513	219	513	469
NEtFOSA	526	169	526	219
8:2 FTS	527	81	527	507
9Cl-PF3ONS	531	351	533	353
PFNS	549	80	549	99
PFUnA	563	269	563	519
NMeFOSAA	570	419	570	483
NEtFOSAA	584	419	584	526
PFDS	599	80	599	99
PFDOA	613	319	613	569
NMeFOSE	616	59		
NEtFOSE	630	59		
11Cl-PF3OUdS	631	451	633	453
PFTrDA	663	169	663	619
PFDoS	699	80	699	99
PFTeDA	713	169	713	669

Quantification is based on response from transition corresponding to Parent 1 > Daughter 1. Secondary transition is used for qualitative identification.

Trace Analysis Summary

The third table (figure 3) is summary of the trace analysis. We have color coded the columns to help explain the table. The columns will be uncolored in your data packet.

Figure 3: Trace Analysis Summary

	Reporting Limit (%wt)	LOQ (ng/g)	Measured Conc (ng/mL)	Dilution factor	% Composition
PFHxS	**0.05**	**0.01**	**2.40**	**100**	**99.45**
PFPeS	**0.05**	**0.01**	**0.73**	**1**	**0.30**
PFOA	**0.10**	**0.01**	**0.25**	**1**	**0.10**
PFBS	**0.05**	**0.01**	**0.17**	**1**	**0.07**
6:2 FTS	**0.05**	**0.05**	**0.14**	**1**	**0.06**
PFBA	0.10	0.01	0.04	1	<0.1
PFMPA	0.10	0.05	N.D.	1	<0.1
3:3FTCA	0.10	0.03	N.D.	1	<0.1
PFPeA	0.10	0.06	N.D.	1	<0.1
PFMBA	0.10	0.03	N.D.	1	<0.1
HFPO-DA	0.10	0.03	N.D.	1	<0.1
NFDHA	0.10	0.05	N.D.	1	<0.1
PFHxA	0.10	0.20	N.D.	1	<0.1
PFEESA	0.10	0.01	N.D.	1	<0.1
4:2 FTS	0.10	0.02	N.D.	1	<0.1
5:3FTCA	0.05	0.05	N.D.	1	<0.05
PFHpA	0.10	0.31	N.D.	1	<0.1
ADONA	0.10	0.01	N.D.	1	<0.1
7:3 FTCA	0.10	0.05	<LOQ	1	<0.1
PFHpS	0.10	0.31	N.D.	1	<0.1
PFNA	0.05	0.01	N.D.	1	<0.05
PFOS	0.05	0.06	N.D.	1	<0.05
FOSA	0.13	0.02	N.D.	1	<0.125
NMeFOSA	0.13	0.01	N.D.	1	<0.125
PFDA	0.10	0.01	N.D.	1	<0.1
NEtFOSA	0.10	0.01	N.D.	1	<0.1
8:2 FTS	0.05	0.05	N.D.	1	<0.05
9Cl-PF3ONS	0.05	0.05	<LOQ	1	<0.05
PFNS	0.05	0.01	<LOQ	1	<0.05
PFUnA	0.10	0.01	N.D.	1	<0.1
NMeFOSAA	0.13	0.01	N.D.	1	<0.125
NEtFOSAA	0.13	0.01	N.D.	1	<0.125
PFDS	0.05	0.01	N.D.	1	<0.05
PFDOA	0.10	0.03	N.D.	1	<0.1
NMeFOSE	0.13	0.09	N.D.	1	<0.125
NEtFOSE	0.13	0.08	<LOQ	1	<0.125
11Cl-PF3OUdS	0.05	0.05	N.D.	1	<0.05
PFTrDA	0.10	0.38	N.D.	1	<0.1
PFDoS	0.05	0.01	N.D.	1	<0.05
PFTeDA	0.10	0.025	N.D.	1	<0.1

🟥 **Reporting Limit:** Typically, 0.05% for sulfonates, 0.10% carboxylic acids, and 0.125% for sulfonamides.

🟦 **LOQ:** Limit of Quantitation (LOQ) of the instrument. Value is equal to the lowest calibrator or the batch specific MDL, whichever is greater.

🟩 **Measured Conc:** Measured concentration on instrument. <LOQ means the peak was detected but below the analyte's LOQ. Not Detected (N.D.) analyte was below the detection limit of the instrument.

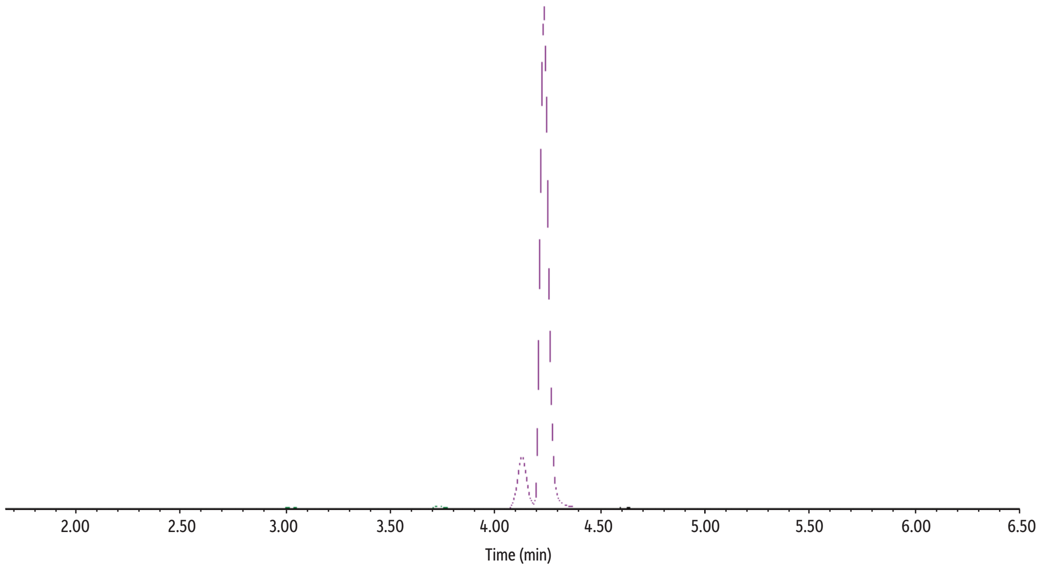
🟧 **Dilution factor:** The dilution factor each analyte was quantified from. Target analyte typically had to be diluted to ensure the measured concentration was within the linear range of the analyte.

🟪 **% Composition:** Results in % wt for each target analyte. Values are calculated from Measured Concentration * Dilution Factor. Final values are normalized to 100%. Reporting limits are applied after normalization.

Overlay MRM Chromatogram

The next data (figure 4) is an overlay MRM chromatogram of the trace analysis. The full scan data can be found in the CofA. The data is typically from the most concentrated value measured.

Figure 4: Overlay MRM Chromatogram



NMR Analysis to Identify Individual Isomers

NMR Table

The fourth table (figure 5) includes NMR data, which lists sample preparation information and summary of results.

Figure 5: NMR Table

NMR
NMR Isomeric ratios determined by NMR will differ from ratios determined chromographically due to unresolved separation. Identification of individual isomers is based on published work. (doi: 10.1016/j.chemosphere.2007.06.096) Samples were prepared at approximately 10mM with an approximate MDL of 1%wt.
Summary of Results
Identified the following isomers: 1-m, 2-m, 3-m, 4-m, and 3,3-dm.

In the Summary of Results, the number denotes distance from end-functional group. *M* stands for "methyl" and dm for "dimethyl," indicating the isomer contains either a single-branching CF_3 group or two CF_3 groups respectively.

Figure 6: Example Numbering Convention for PFAS Isomers

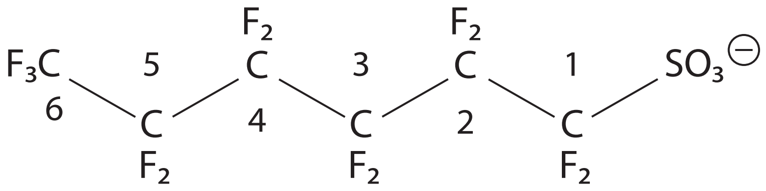
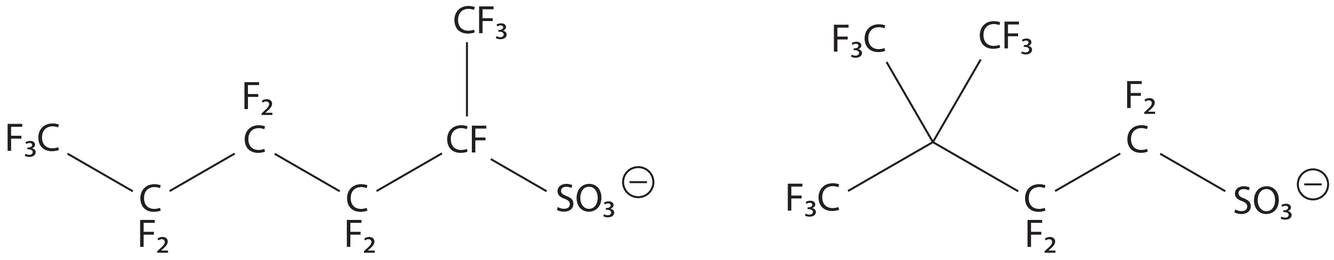


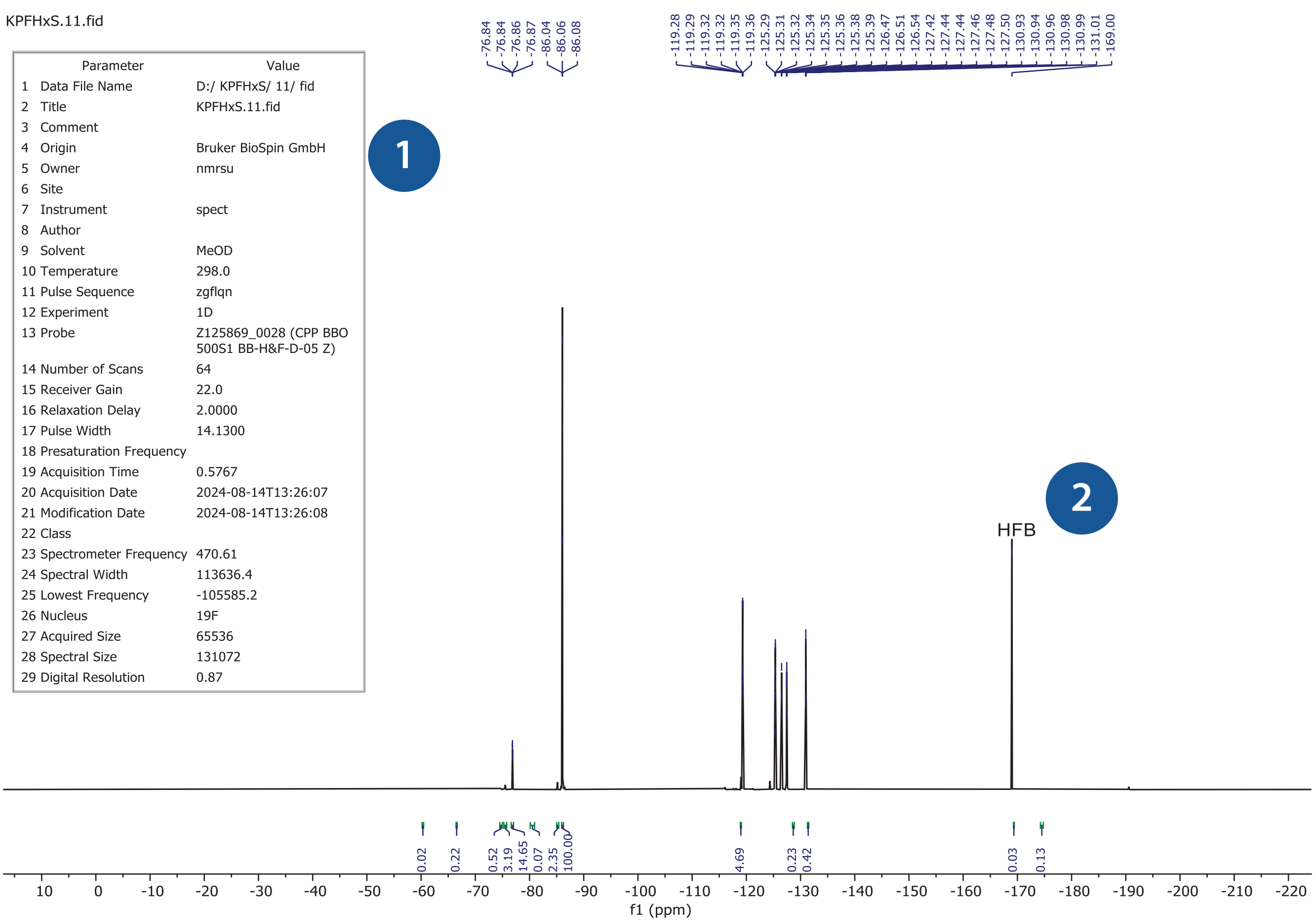
Figure 7: Example Isomer Naming Convention



NMR Data

The final data (figure 8) included in the trace analysis data packet is additional NMR data.

Figure 8: NMR Data-Annotated



KPFHxS.11.fid

	Parameter	Value
1	Data File Name	D:/ KPFHxS/ 11/ fid
2	Title	KPFHxS.11.fid
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Instrument	spect
8	Author	
9	Solvent	MeOD
10	Temperature	298.0
11	Pulse Sequence	zgflqn
12	Experiment	1D
13	Probe	Z125869_0028 (CPP BBO 500S1 BB-H&F-D-05 Z)
14	Number of Scans	64
15	Receiver Gain	22.0
16	Relaxation Delay	2.0000
17	Pulse Width	14.1300
18	Presaturation Frequency	
19	Acquisition Time	0.5767
20	Acquisition Date	2024-08-14T13:26:07
21	Modification Date	2024-08-14T13:26:08
22	Class	
23	Spectrometer Frequency	470.61
24	Spectral Width	113636.4
25	Lowest Frequency	-105585.2
26	Nucleus	19F
27	Acquired Size	65536
28	Spectral Size	131072
29	Digital Resolution	0.87

Figure annotations:

1. Acquisition parameters for NMR data.
2. Hexafluorobenzene (HFB) added as an internal standard to determine relative chemical shifts.

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