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Ensuring Data Quality by Benchmarking System Performance Using Waters Neutrals Quality Control Reference Material

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Abstract

This application note focuses on how the standard can be used to benchmark and monitor system performance over the life of the system. By using the reference standard to benchmark system performance, data integrity can be monitored and assured.

Benefits

- Reliably benchmark system performance using a strictly manufactured and certified reference standard
- Monitoring system performance can help prevent the collection of inaccurate data
- Detects system problems before they happen, potentially reducing instrument downtime

Introduction

Regardless of what industry a chromatographer works in, system performance and data reliability are of the utmost importance. If a system's performance starts to decline, the reliability and accuracy of the data could be in question. Furthermore, if a system's performance drops too much, system repairs might be in order, resulting in instrument downtime and reduction of productivity in the lab. By routinely monitoring system performance,

however, a drop in performance can be observed earlier and corrective action can be taken, potentially reducing system downtime and preventing erroneous data from being collected. One way to monitor system performance is to benchmark the system using a system suitability standard, and then compare subsequent runs of the standard to the benchmarked data to ensure that the system is performing reliably.

Waters Neutrals Quality Control Reference Material (QCRM) is a mixture of three neutral compounds that are an ideal system reference standard. The use of neutral compounds allow the QCRM to be unaffected by mobile phase pH, making it compatible with buffered and non-buffered mobile phases at both high and low pH. Thus, the standard can be analyzed on many different HPLC and UHPLC systems, with different column chemistries, and different mobile phases. The highly controlled manufacturing process of the standard ensures a high quality and reliable standard that can be counted on to produce consistent results over time. This application note focuses on how the standard can be used to benchmark and monitor system performance over the life of the system. By using the reference standard to benchmark system performance, data integrity can be monitored and assured.

Experimental

ACQUITY UPLC H-Class Conditions

Mobile phase:	50:50 acetonitrile: water
Separation mode:	Isocratic
Detection:	UV 254 nm
Column:	ACQUITY UPLC BEH C_{18}, 2.1 x 50 mm 1.7 µm
Column temp.:	30 °C
Needle wash:	50:50 ACN:water
Sample purge:	50:50 ACN:water

Seal wash:	50:50 MeOH:water
Flow rate:	0.6 mL/min
Injection volume:	1 µL
Data management:	Empower 3 CDS
Sample preparation	A vial of Neutrals QC Reference Material (PN: 186006360) was opened and transferred into an LCGC Certified Clear Qsert Vial (PN:186001126C) for injection.

Results and Discussion

System performance and data reliability are something that every chromatographer should be conscious of. A system should be monitored regularly to ensure that it is continually performing at an optimum level to generate quality data. The easiest way to evaluate system performance is to routinely use a QCRM standard to benchmark the system when it is performing optimally. At later dates, subsequent injections of standard can be compared to the original data to ensure that the system is still performing well. Waters Neutrals QC Reference Material (NQCRM) is a mixture of three neutral compounds: acetone, naphthalene, and acenaphthene. The separation of these compounds is achieved under common mobile phase conditions with sufficient organic content. Figure 1 shows the isocratic separation of the Neutrals QCRM on an ACQUITY UPLC BEH C_{18} 2.1 x 50 mm 1.7 µm Column with 50% acetonitrile in water as the mobile phase.

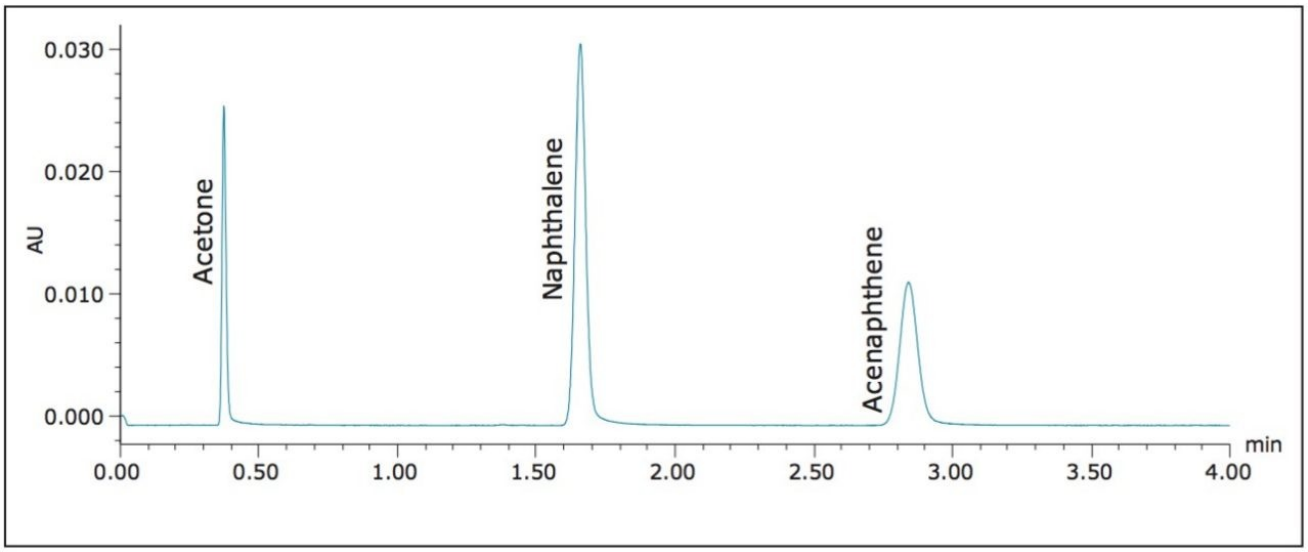

Figure 1. Sample chromatogram of the Waters Neutrals QCRM separation on an ACQUITY UPLC BEH C_{18} , 2.1 x 50 mm 1.7 µm Column.

In this application, the standard was used to benchmark the system performance of an ACQUITY UPLC H-Class System equipped with a PDA detector for a period of five days (120 h). Prior to beginning the experiment, the system was calibrated and performance maintenance was performed to ensure proper operation of the system. Benchmarking a system that is not performing optimally could lead to irregular and unreliable benchmarking results. The Neutrals QCRM was injected in triplicate onto an ACQUITY UPLC BEH C_{18} , 2.1 x 50 mm, 1.7 µm Column three times a day for five days. The first set of injections was performed in the morning, the second at mid-day, and the third in the late afternoon to simulate the standard being run before, during and after an eight-hour shift. A total of 45 injections were performed over five days (120 h). Retention time, USP tailing factor, and system pressure were monitored. These parameters were monitored since they are typically parameters that could indicate a serious system problem. If, for instance, the retention time of the peaks changed significantly, it could indicate a pump issue or an error in mobile phase preparation; while an increase in USP Tailing Factor could indicate a failing column or that the column outlet fitting is not seated properly.[1]

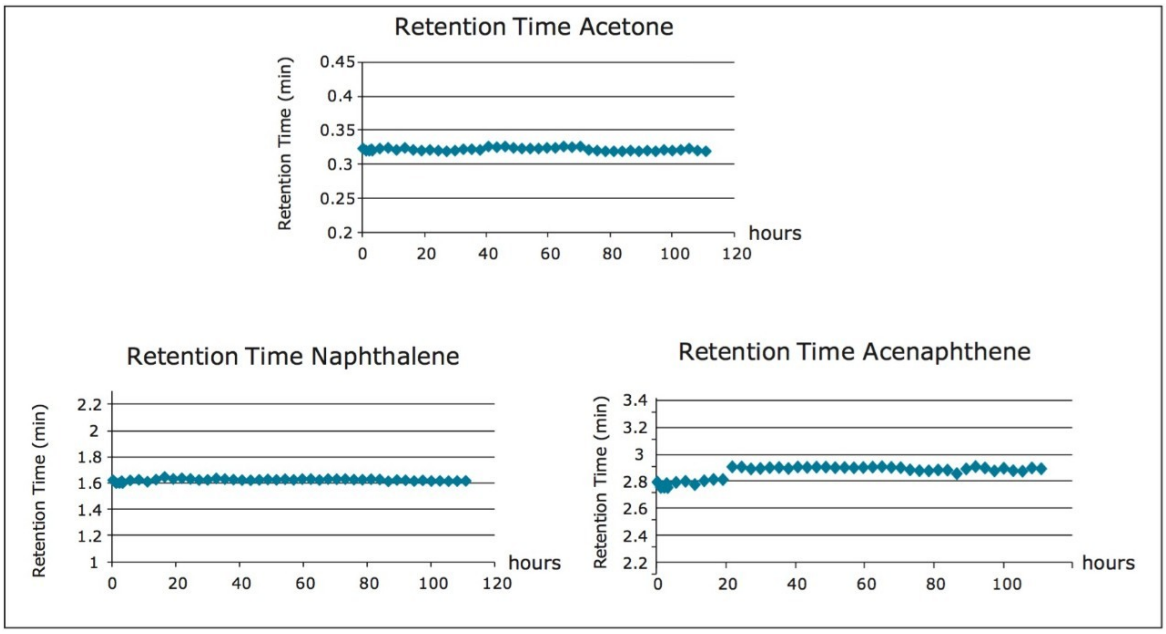

Figure 2. Retention time trending data for the Neutrals QCRM over five days (120 h).

As the trending data shows, the Neutrals QCRM is a valuable tool for benchmarking a system's performance. The data shows the high reproducibility of the system over time, with a retention time %RSD < 0.7 for all three peaks in the Neutrals QCRM standard, as shown in Table 1. The trending data for the USP tailing factor shows very little deviation over the course of the analysis, indicating that the peaks are not changing over time. The system pressure trending data shows very little variation as well, displaying a stable pressure over the course of the experiment. In this experiment, the monitoring of retention time, USP tailing factor, and system pressure was important, since any change in these parameters could indicate a system or column problem, and potential collection of erroneous data for experiments run on the system over these five days.

	Average Retention Time (min)	%RSD Retention Time
Acetone	0.323	0.69
Naphthalene	1.633	0.44
Acenaphthene	2.893	0.44

Table 1. System performance benchmarking data using the Waters Neutrals QCRM, showing highly reproducible retention times demonstrated by low %RSD (n=45) over five days (120 h).

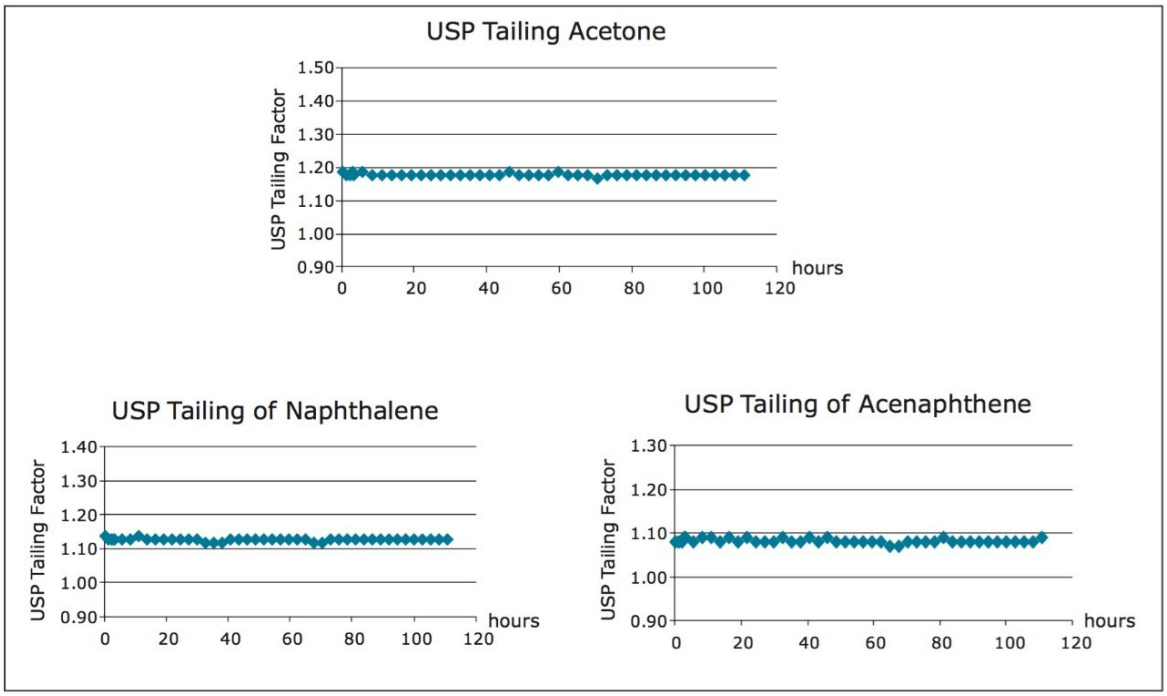

Figure 3. USP tailing factor trending data for the Neutrals QCRM over five days (120 h).

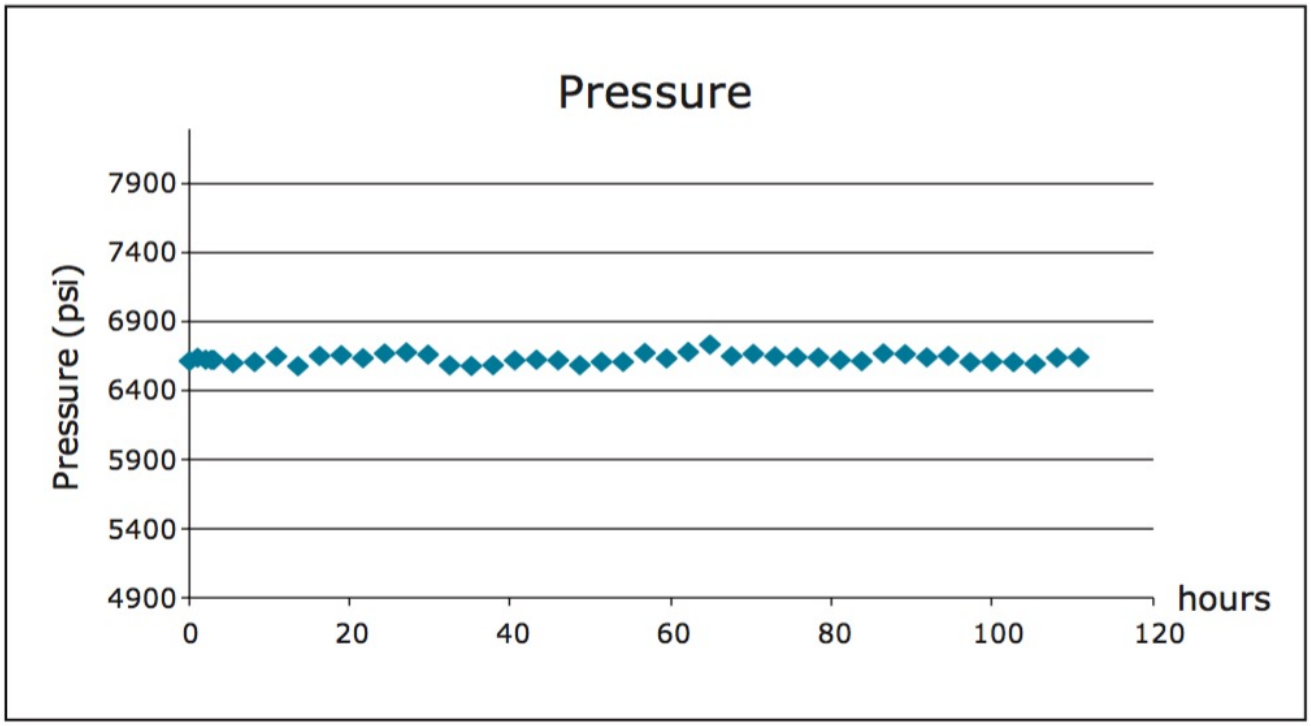

Figure 4. System pressure trend plot of the Neutrals QCRM indicating consistent system pressure over time.

In addition to monitoring system performance, this data 'benchmarks' a starting point that future injections of the Neutrals QCRM can be compared to. After gathering the benchmark data, a set of specifications can be created to monitor the system.[2] After these specifications are created, the QCRM can be run periodically and checked

against these specifications to determine if the system is still operating optimally. If the Neutrals QCRM falls out of specification, the system may need to be repaired. After these repairs are completed, the Neutrals QCRM can be run again and the data can be compared to the specifications to see if the system is working properly.[1]

Conclusion

Monitoring system performance is an important aspect of liquid chromatography that should be performed routinely to ensure the highest quality data generated. Routinely monitoring a system with a well-characterized and controlled standard can lead to early detection of system problems, potentially reducing system downtime. Using Waters Neutrals QC Reference Material (QCRM) is an ideal way to benchmark an optimally functioning system. Waters Neutrals QCRM is a mixture of three neutral compounds that can be separated using a wide variety of column chemistries and mobile phases, making it compatible with most methods and laboratory practices. Once the system has been benchmarked, the Neutrals QCRM can be run on a regular basis and compared to a set of specifications that the operator creates to ensure that the system is still working optimally. If the system is outside of specification, corrective action can be performed before erroneous data is collected or the system fails. Using the Neutrals QCRM to benchmark system performance can lead to reduced system downtime and the efficient acquisition of reliable data, saving considerable time and resources in the laboratory.

References

1. Berthelette KD, Summers M, Fountain KJ. Troubleshooting Common System Problems using Waters Neutrals QC Reference Material. Waters Application Note
2. Quality Control Reference Material and Benchmarking Instrument Performance. Waters White Paper.

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- ACQUITY UPLC H-Class PLUS System <https://www.waters.com/10138533>
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