How to Choose the Proper SPME Fiber

The most common question we receive concerning SPME is, naturally, “Which fiber should I use for extracting my specific analyte?” Recently, we evaluated the abilities of currently available SPME fibers to extract organic analytes of various classes and molecular weights. From the results, we hoped to make some general recommendations.

First we focused on volatile analytes with similar size (molecular weight 58-89) and structure, but different functionalities (Table 1). We introduced these analytes into water at 1ppm each, extracted them, using 6 different fibers, then determined absolute responses for each analyte, extracted by each fiber. Table 1 lists the best fibers for extracting each of these analytes. Where possible, the three best choices are given.

For extracting analytes with molecular weights of less than 90, regardless of functionality, the clear choice is the 85µm Carboxen™/polydimethylsiloxane (PDMS) StableFlex™ fiber. For nearly all of

(continues on page 2)
these analytes, responses for the Carboxen/PDMS fiber were more than 100 times greater than responses for any other fiber. Apparently, the porous Carboxen particles retain any small analyte that comes in contact with the pores. The Carboxen/PDMS fiber extracts these analytes by adsorption, as opposed to absorption, the extraction mechanism of fibers coated solely with liquid phase. The only analyte that did not follow the pattern was isopropylamine. Divinylbenzene (DVB) fibers have a high affinity for small amines. Consequently, the combination coating of DVB over Carboxen was the best choice for isopropylamine. However, the Carboxen/PDMS fiber and the PDMS/DVB fiber also were suitable for extracting isopropylamine.

Next, we extracted larger analytes, again from varied organic classes (Table 1). We introduced these analytes into water at 75 ppb each, extracted them at 3 pH levels, using 8 coated and uncoated SPME fibers, analyzed the extracts by GC/MS, and compared the absolute response for each analyte extracted by each fiber at each pH.

Unlike the results for the volatile analytes, often there was no clear choice of SPME fiber for a particular larger analyte (Table 1). Because liquid phases can retain larger analytes as effectively as porous materials, the effect of polarity was not as great. For larger analytes, the effect of polarity becomes more significant. Both Carbowax/DVB and polyacrylate (PA) fibers were suitable for polar analytes. The DVB/Carboxen fiber also was excellent for extracting many of the higher molecular weight analytes; larger analytes concentrate in the DVB layer and smaller analytes concentrate in the Carboxen layer. For some analytes, such as dimethylphthalate and N-nitrosodi-n-butylamine, there were more than three choices: all of the DVB-containing fibers, the PA fiber, the Carboxen fiber, and the 100µm PDMS fiber were suitable.

A surprising result was the ability of polyacrylate (PA), a fairly polar fiber, to extract nonpolar analytes, apparently through pi bonds. The results also indicate that Carboxen does not easily desorb larger analytes, particularly PAHs. It is interesting that the Carboxen fiber was effective for extracting decachlorobiphenyl. Perhaps the large chlorine groups prevent the molecule from becoming too tightly attached to the Carboxen particles. These latter observations point out that generalizations can be made concerning fiber selection, but ultimately the best fiber for a particular application should be determined by testing.

For a complete report on this investigation of fiber choice to a specific analyte, request a copy of Bob Shirey’s 1999 EAS paper entitled Selecting the Appropriate SPME Fiber for Your Application Needs (T499232). Use the reply card on page 4 of this newsletter.
Upcoming Exhibits

Water Quality Conference (WQT)
Tampa, FL, Oct. 31-Nov. 2

New AWWA Method 6040, for determination of odors in drinking water by SPME, is currently under review by the AWWA odor committee. Method 6040 simplifies the determination of odor concentration at a less costly approach than traditional closed-loop stripping techniques. Stop by Supelco Booth #304 and ask about our new odor and carbamate standards for drinking water analysis. Also, request your free copy of the new SPME Application Guide, a compilation of literature references for nearly 400 technical articles on SPME.

Eastern Analytical Symposium (EAS)
Somerset, NJ, Nov. 15-18

- Stop by Supelco Booth #318 to discuss your SPME application.
  While visiting, pick up a copy of the SPME Applications Guide.
- Be sure to attend the SPME Symposium, Advances in Solid Phase Microextraction, on Tuesday Morning, Nov. 16. Following is a list of the scheduled talks.

  10:20am Break
  10:40am  Forensic and Toxicology Applications: Accelerants, Explosives and Drug Analysis by SPME. José R. Almirall, Dept. of Chemistry and The International Forensic Research Institute, Florida International University, University Park, Miami, FL 33199.
  11:00am  Use of SPME Fibers for Measurement of Vapor Signatures of Buried Landmines. Thomas F. Jenkins, U.S. Army Cold Regions Research and Engineering Laboratory, 72 Lyme Rd., Hanover, NH 03755 and Thomas A. Ranney, Science and Technology Corporation, 72 Lyme Rd., Hanover, NH 03755.
  11:40am  Applications of SPME in Personal Care Product. Richard K. Payne, Colgate-Palmolive Co., Corporate Research Center, 909 River Road, Piscataway, NJ 08855-1343.
New Products

Products for Odor Determination in Drinking Water

**50/30µm Divinylbenzene/Carboxen/PDMS Stableflex Fibers**
For manual sampling. 2cm fiber length.  
Cat. No. 57348-U

**40mL Vial Holder**
Five-position holder for headspace sampling of volatiles and odors. The aluminum block is used for heating and stirring in SPME headspace extractions.  
Cat. No. 33313-U

**40mL Headspace Vials**
Clear glass, 29 x 81mm.  
Pack of 100.  
Cat. No. 27184

**StableFlex™ Coated SPME Fibers Exhibit the Same Performance as Our Original Fibers, But with Less Breakage**
Many of our SPME fibers now are available with a coating of StableFlex material. StableFlex fibers are more flexible than our original fibers, and are much less likely to break. StableFlex fibers also exhibit longer lifetime (more injections can be made on a single fiber), greater stability, and less bleed.

Choose StableFlex SPME fibers with either a standard needle (24 gauge) or with a 23-gauge needle (for use with the Merlin Microseal™ sealing system for a proper seal with Microseal septa). Fiber length 1cm unless otherwise indicated. Sold in packs of 3.

<table>
<thead>
<tr>
<th>StableFlex SPME Fiber Assemblies¹</th>
<th>For Manual Sampling</th>
<th>For Automated Sampling² or HPLC</th>
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<tr>
<td></td>
<td>Standard Needle</td>
<td>23 Gauge Needle</td>
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<tr>
<td>65µm Polydimethylsiloxane/Divinylbenzene (PDMS/DVB)</td>
<td>$160.00</td>
<td>$170.00</td>
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<tr>
<td>Ideal for many polar analytes, especially amines.</td>
<td>57326-U</td>
<td>–</td>
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<tr>
<td>85µm Carboxen/Polydimethylsiloxane (CAR/PDMS)</td>
<td>$160.00</td>
<td>$170.00</td>
</tr>
<tr>
<td>Ideal for gaseous/volatile analytes, high retention for trace analysis.</td>
<td>57334-U</td>
<td>–</td>
</tr>
<tr>
<td>70µm Carbowax/Divinylbenzene (CW/DVB)</td>
<td>$160.00</td>
<td>$170.00</td>
</tr>
<tr>
<td>For polar analytes, especially for alcohols, low temperature limit.</td>
<td>57336-U</td>
<td>57338-U</td>
</tr>
<tr>
<td>50/30µm Divinylbenzene/Carboxen/PDMS (DVB/CAR/PDMS)</td>
<td>$160.00</td>
<td>$170.00</td>
</tr>
<tr>
<td>Ideal for broad range of analyte polarities, good for C3-C20 range.</td>
<td>57328-U</td>
<td>–</td>
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<td>57348-U³</td>
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¹ Requires an SPME fiber holder (see the Supelco catalog).
² Use with AutoSampler requires Varian SPME upgrade kit (available from Varian).
³ 2cm fiber.

To Order:
Phone 800-247-6628 or 814-359-3441
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