

## Headspace vials:

### Round bottom or flat bottom?

Choosing a headspace vial with a flat (also called square) bottom or round bottom depends on your particular instrument. Generally, round bottomed vials are used for robotic arm autosamplers that will pickup a vial and bring it to the autosampler needle, while flat bottomed vials are used for autosamplers that bring the needle to the vial.

A round bottom vial is self aligning when it's returned to the vial rack by the robotic arm, while a flat bottomed vial is slightly more stable while it's in the rack.

It is best to check your autosampler's user manual if you are not sure.

### Beveled or flat top?

Flat topped vials can be used with almost any headspace autosampler. Beveled top vials can be used with some autosamplers. As usual, the best way to be sure which to choose is to check your autosampler's manual. A quick guideline is that autosamplers that don't move the vial out of the rack can use beveled top vials. Robotic arm autosamplers that use a magnetic pick-up must use flat top vials (to give adequate contact between the magnet and the cap). Other robotic arm autosamplers may or may not be able to use beveled top vials, depending on how they grip the vial.

Beveled top vials can improve the seal formed by the crimp top. In a flat topped vial, the sealing pressure is primarily at the outer rim of the vial, cap and septum. With a beveled top vial, the sealing pressure is evenly distributed across the top of the vial, improving the seal.

### Screw-top or crimp-top?

Screw caps for headspace vials are a recent development, originally intended for magnetic robotic arm autosamplers.

They side step the problem of crimping on an all-steel cap or a composite steel / aluminium cap.

The plated steel caps are reusable, and do not require tools to seal or open vials. They have some drawbacks too. They can only be used for 10mL and 20mL vials. Too much of the internal volume of a 6mL vial is lost to the threaded neck for the cap. Screw cap headspace vials are not suitable for use with mechanical robotic arm autosamplers. The neck of a screw thread vial is a different diameter than that of a crimp top vial, and the screw cap vial lacks the natural ledge formed by lip of a crimp top vial. That ledge is frequently used by the autosampler to help align and lift the vial.



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