



Best Practices for Limiting Hazardous Solvent Exposure with SafetyCaps and Waste Containment for HPLC and UHPLC Systems

Webinar Outline

Introducing MAC-MOD SafetyCaps and SafetyWasteCaps

Review of Hazardous Chemicals used in
Chromatography Labs

Mobile Phase Solvent Containment

Waste Solvent Containment

Case Studies I & II



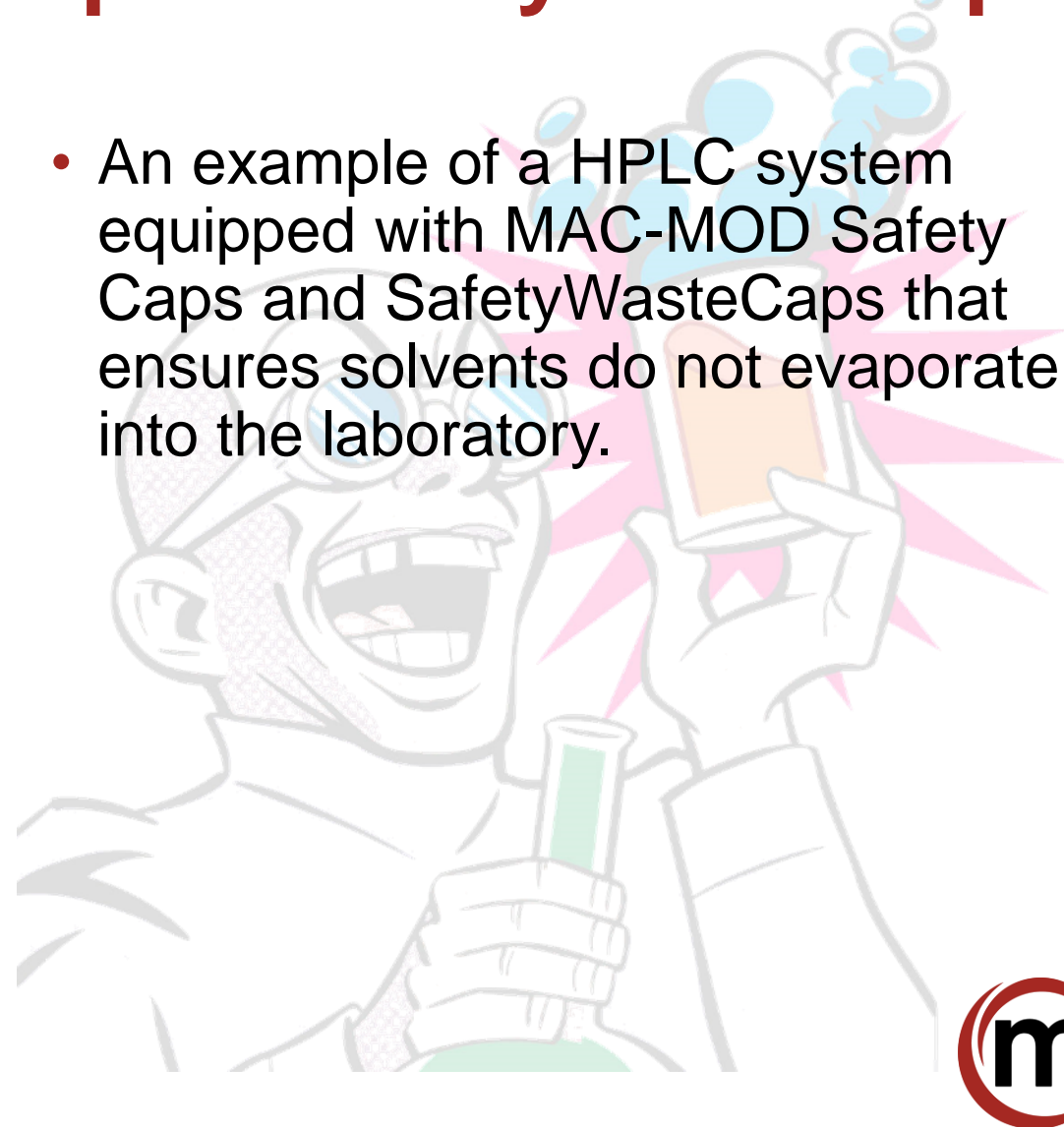
Why should I implement MAC-MOD SafetyCaps in my lab?



What is a MAC-MOD SafetyCap or SafetyWasteCap?



- An example of a HPLC system equipped with MAC-MOD SafetyCaps and SafetyWasteCaps that ensures solvents do not evaporate into the laboratory.



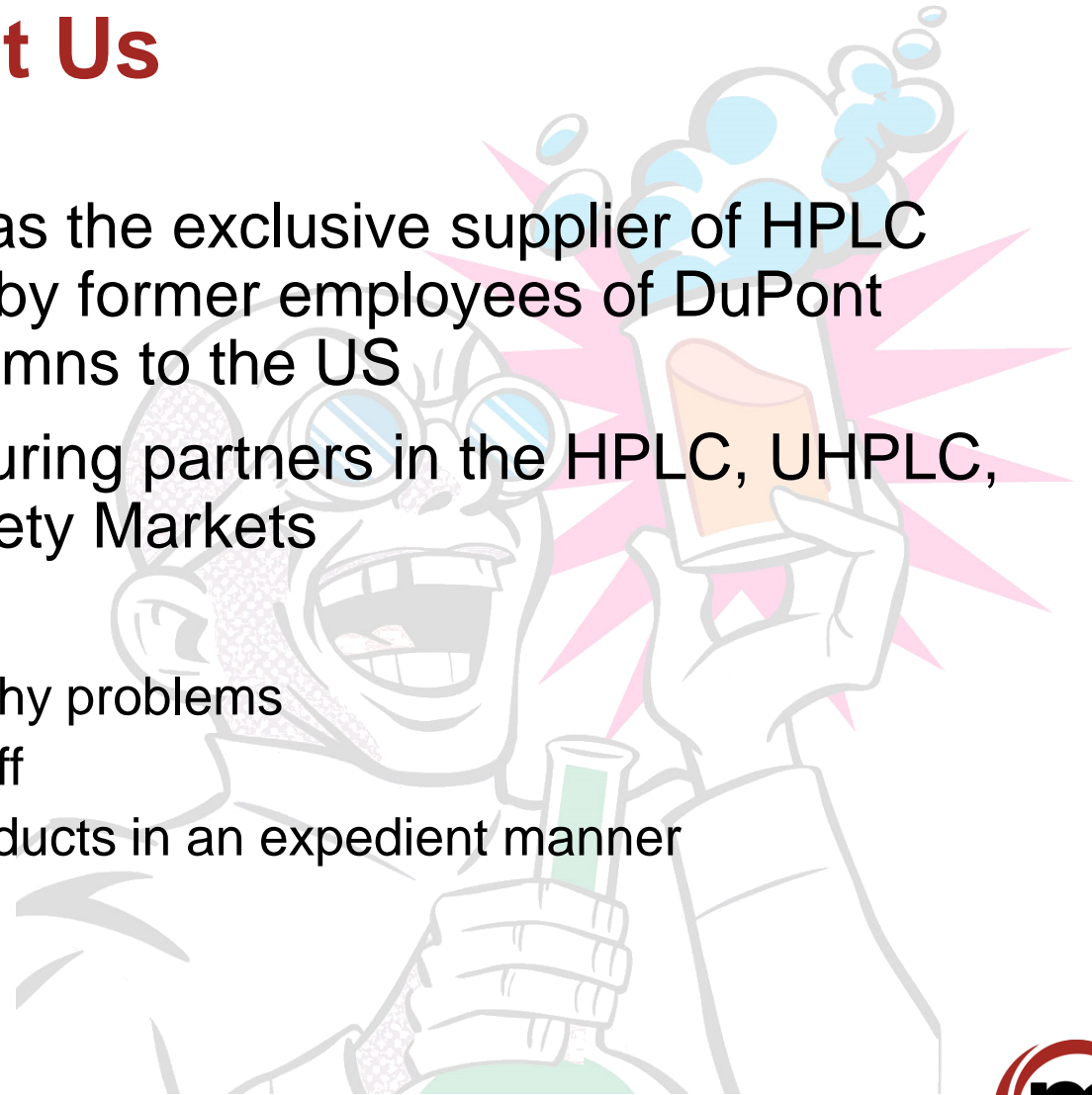
When and where was the MAC-MOD SafetyCap developed?

- Founded in 1998 in Kelsterbach, Germany by the Safety Center for Analytical Technologies (S.C.A.T.).
- Known for introducing the first commercially available hermetically sealed mobile phase closure system
- Distributed by MAC-MOD Analytical in the US



MAC-MOD Analytical - About Us

- Founded in 1986 in Chadds Ford, PA as the exclusive supplier of HPLC columns from Rockland Technologies by former employees of DuPont Company selling **ZORBAX** HPLC columns to the US
- Currently represent multiple manufacturing partners in the HPLC, UHPLC, Chromatography Accessories and Safety Markets
- Capabilities
 - Ability to solve complicated chromatography problems
 - Technically focused sales and support staff
 - Maintain excellent inventory to supply products in an expedient manner



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Most Commonly Used Organic Solvents

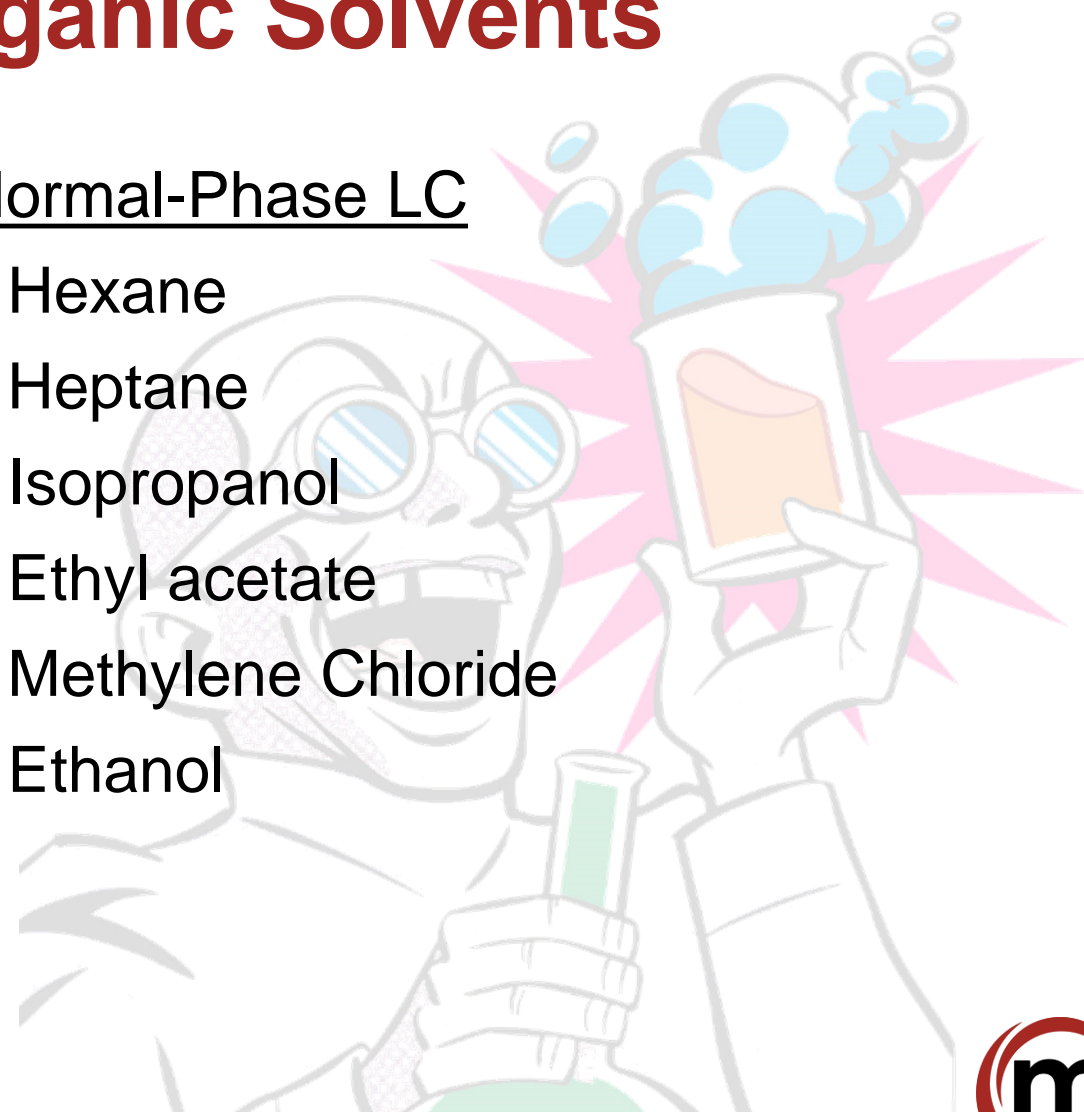
Reversed-Phase LC

- Acetonitrile*
- Methanol
- Isopropanol
- n-Propanol
- Tetrahydrofuran (THF)
- Ethanol

Normal-Phase LC

- Hexane
- Heptane
- Isopropanol
- Ethyl acetate
- Methylene Chloride
- Ethanol

*Most common for HILIC too



Vapor Pressures and Boiling Points for Commonly Used RPLC and NPLC Solvents

Reversed-Phase Solvents

Solvent	Vapor Pressure (torr)	Boiling Point (° C)
Acetonitrile	89	81.6
Methanol	97	64.7
Isopropanol	32	82.3
N-Propanol	15	97.2
THF	142	66.0
Ethanol	44	78.4






Normal-Phase Solvents

Solvent	Vapor Pressure (torr)	Boiling Point (° C)
Hexane	124	68.7
Heptane	35.5	98.4
Isopropanol	32	82.3
Ethyl acetate	73	77.1
Methylene Chloride	350	39.8
Ethanol	44	78.4
Chloroform	158	61.2



Globally Harmonized System

The United Nations' Globally Harmonized System of Classification, Labeling and Packaging of Chemicals (GHS) is a globally uniform system for the classification of chemicals and their labeling on packaging and in safety data sheets.

Solvent Name(s) Chemical Formula	Chapter	Hazard Class	Class Division	Hazard Code	Hazard Statement	Exposure Limit according to TRGS 900
Acetonitrile (ACN) C_2H_3N Cyanomethane Ethyl nitrile Methanecarbonitrile Methyl cyanide	2.6	Flammable liquids	Flam. Liq. 2	H225	Highly flammable liquid and vapour	10 ml/m ³ 17 mg/m ³
	3.1	Acute toxicity (oral)	Acute Tox. 4	H302	Harmful if swallowed	
	3.1	Acute toxicity (dermal)	Acute Tox. 4	H312	Harmful in contact with skin	
	3.1	Acute toxicity (respiratory)	Acute Tox. 4	H332	Harmful if inhaled	
	3.3	Serious eye damage / eye irritation	Eye Irrit. 2	H319	Causes serious eye irritation	
		  GHS02 GHS07				
Methanol (MeOH) CH_4O Carbinol Hydroxymethane Methyl alcohol Methyl hydrate Methyl hydroxide Methyl alcohol Methylol Wood spirit	2.6	Flammable liquids	Flam. Liq. 2	H225	Highly flammable liquid and vapour	200 ml/m ³ 270 mg/m ³
	3.1	Acute toxicity (oral)	Acute Tox. 4	H301	Toxic if swallowed	
	3.1	Acute toxicity (dermal)	Acute Tox. 4	H311	Toxic in contact with skin	
	3.1	Acute toxicity (respiratory)	Acute Tox. 4	H331	Toxic if inhaled	
	3.8	Specific target organ toxicity (single exposure)	STOT SE 1	H370	Causes damage to organs (if swallowed, inhaled / in contact with skin)	
		   GHS02 GHS06 GHS08				

Harmful if Inhaled!!

Toxic if Inhaled!!

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The MAC-MOD Solvent Bottle SafetyCap Solution

The Status Quo



- Harmful vapor emission in the labs
- Safety issues for employees
- Drift in HPLC retention times due to differential solvent loss and possible air impurity contamination
- Lost solvent = Solvent Waste = lost Monies



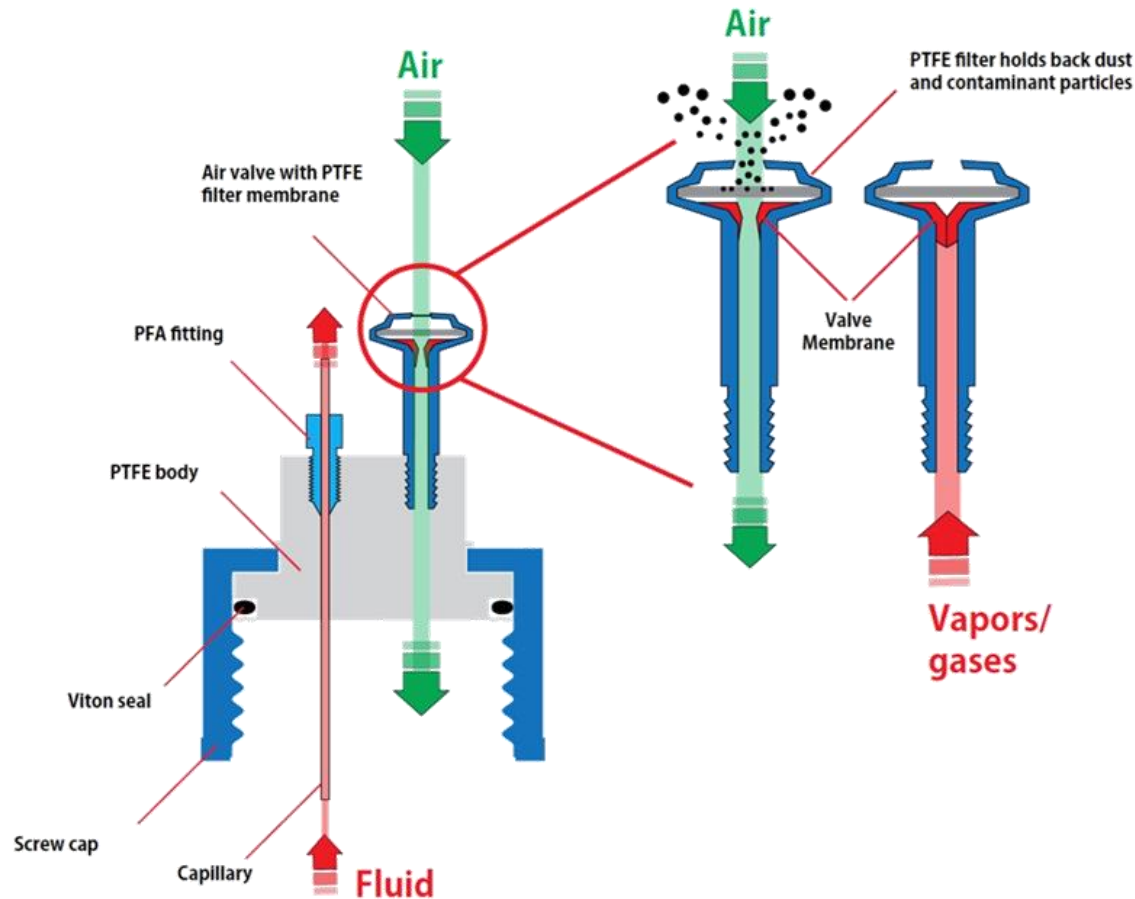
MAC-MOD SafetyCaps A Better Solution



- Hermetically sealed
- No harmful vapors
- Easily change SafetyCaps
- Tubing no longer slips
- Different thread sizes available
- Quick Connect Systems available for ease of use



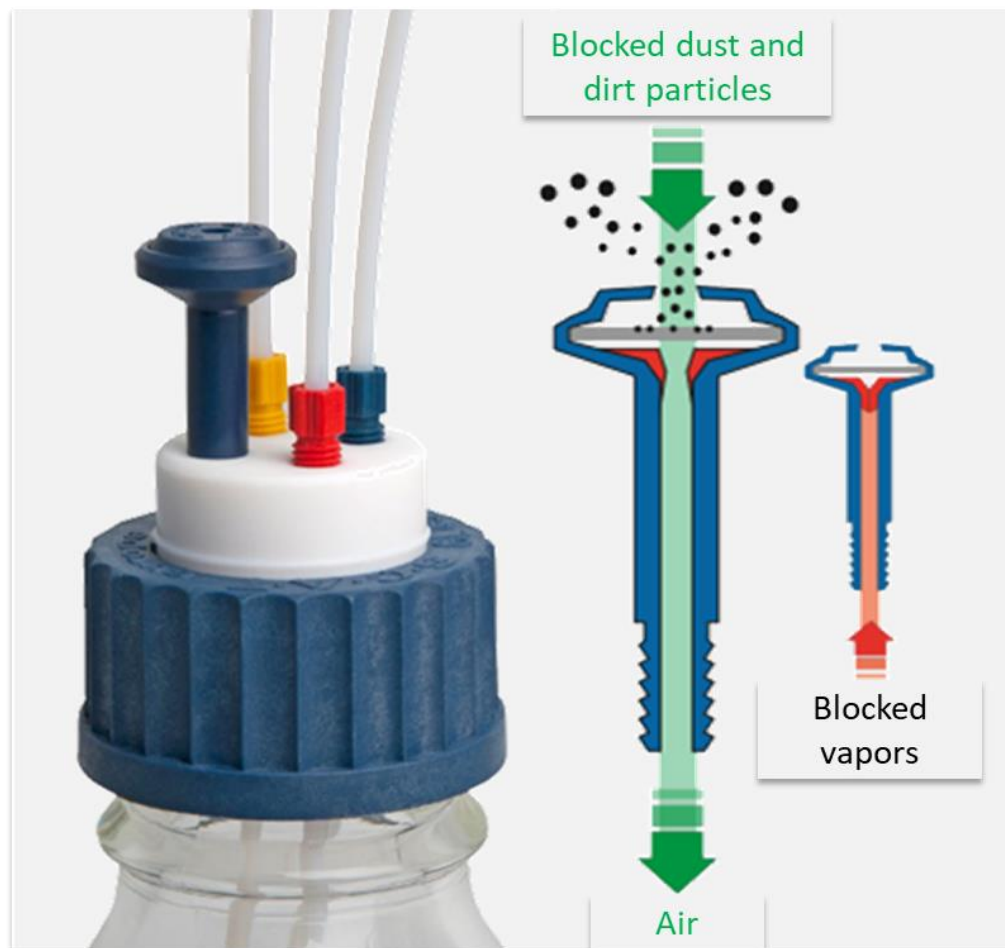
Diagram of the MAC-MOD SafetyCap



- 100% Hermetically Sealed!
- The VITON seal balances the bumps of the glass surface.
- A PTFE covering protects the VITON seal to avoid interaction with the solvents.
- PTFE (Teflon®) is being used for maximum chemical resistance.
- **Freely rotatable cap for easy container exchange** - even with capillaries installed - without twisting or "tangled tubes".
- PFA fittings keep tubes safely fixed and **avoid interruptions caused by air intake** into the HPLC system.
- To prevent vacuum formation in the reservoir as solvent is removed by the pump, an air valve is a key part of each solvent safetycap.



Design and Dynamics of the Air Valve

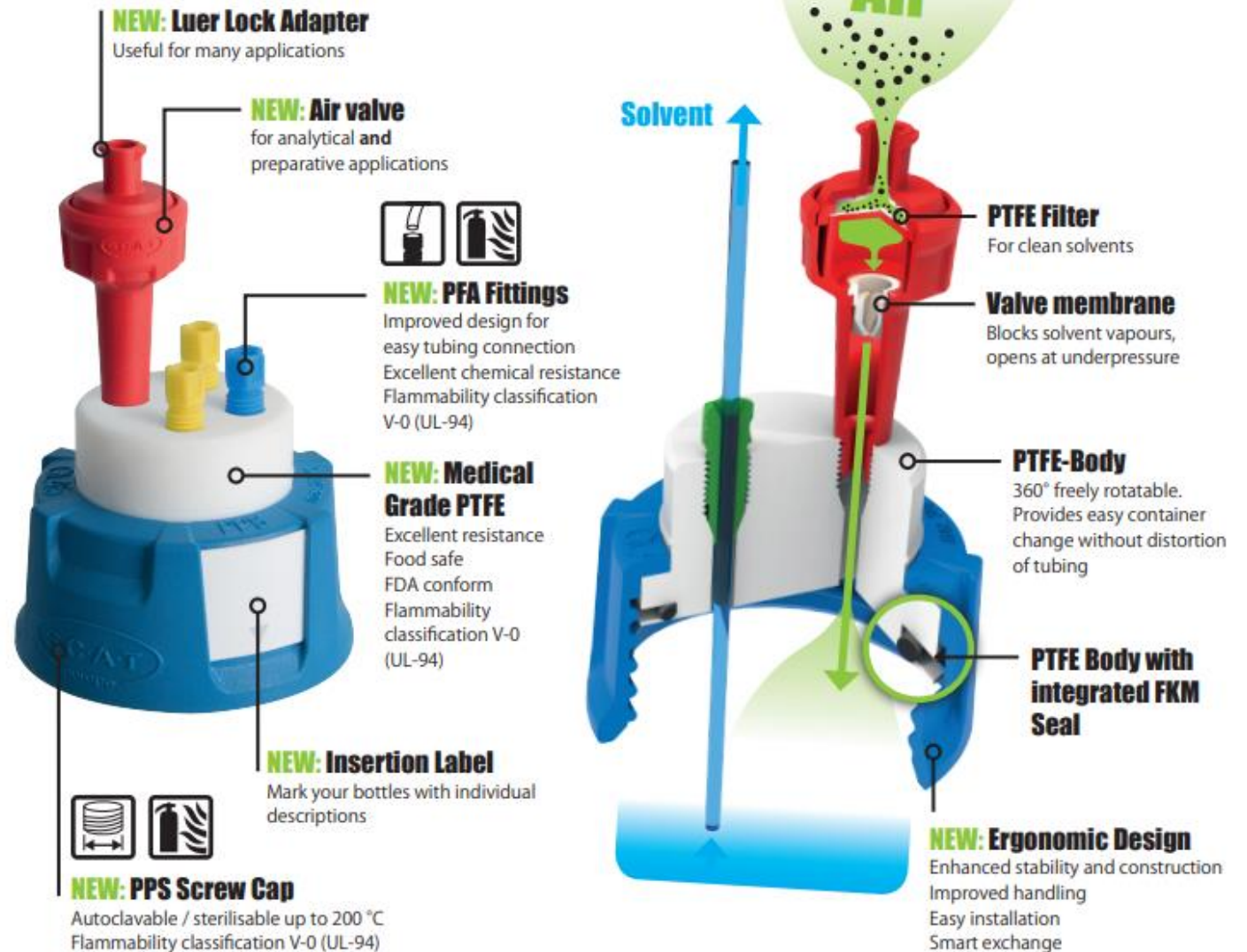


- Pump withdraws solvent from the reservoir, and lab air is filtered as it passes through the air valve.
- The PTFE filter on the air valve **blocks dust and contaminant** particles from the ambient air.
- Air valve **prevents hazardous vapors** from entering the laboratory air and harming employees.
- **No eluent contamination:** results of your analysis remain reproducible.
- Over a period of 6 months, the air valve can **prevent evaporation** of approx. 750 mL of solvent.
- As the filter membrane absorbs contaminants from the ambient air, the valve must be **replaced every 6 months**.
 - **Blue air valve** is designed for a flow rate up to 150 mL/min for conventional applications
 - A new **red air valve** has been designed to replace the original air valve.



MAC-MOD SafetyCaps Version 2.0

- Fire Resistant
- More Durable Body
- Inserted Label for Marking Bottles
- Luer Lock Adapter



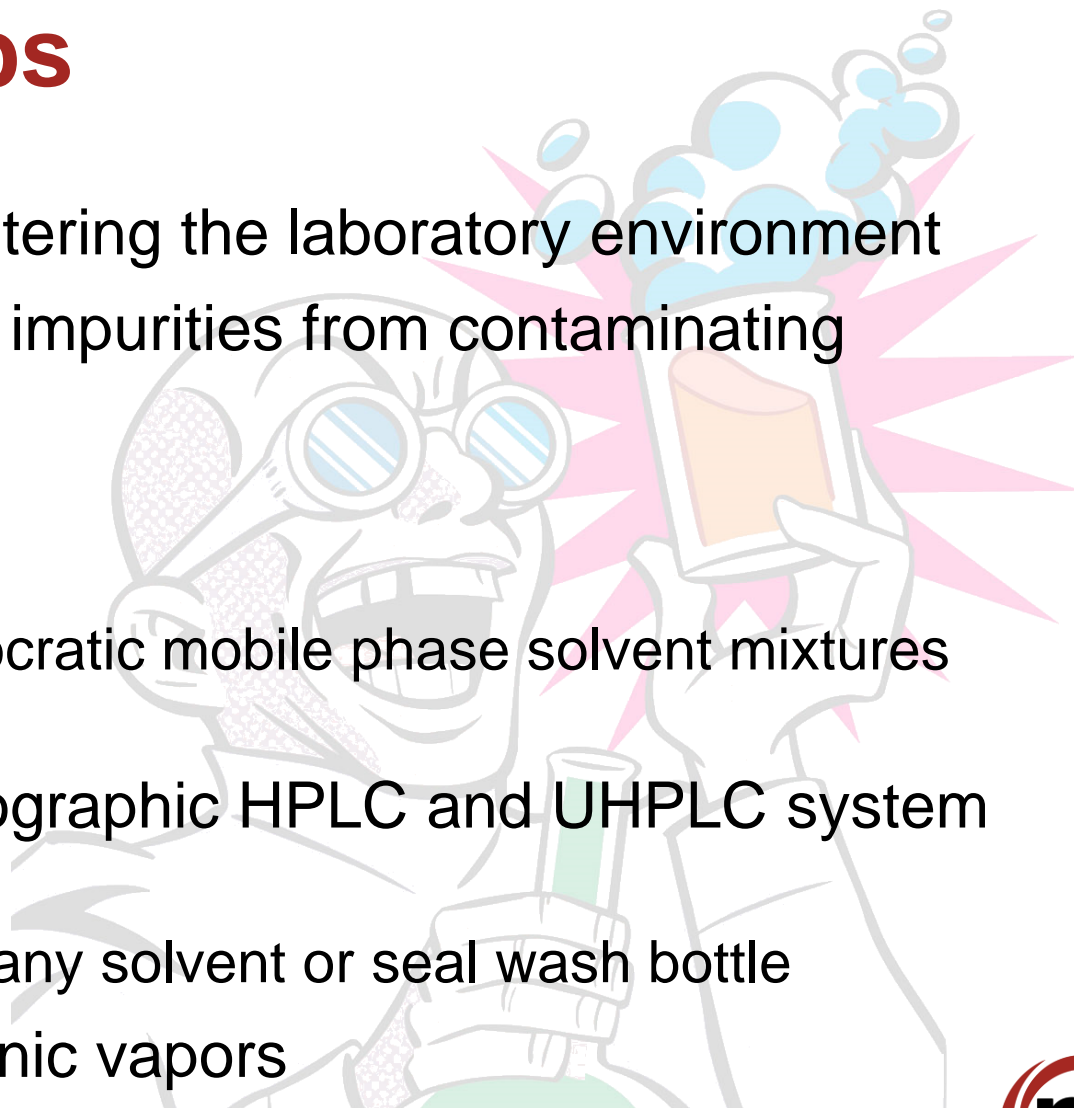
SafetyCap Kits

- All fittings, blind plugs and filters are included
- Easy Storage
- Comes with 4 caps for A,B,C, and D tubing lines



Advantages of SafetyCaps

- Prevent solvent vapors from bottles entering the laboratory environment
- Prevent particulates and laboratory air impurities from contaminating solvents
 - Especially important for LC-MS
- Ensure reproducible analytical results
 - No RT shifts due to ratio changes for isocratic mobile phase solvent mixtures and gradient mobile phase premixes
- Fit every brand and model of chromatographic HPLC and UHPLC system
 - GL45 size cap is the most common
 - Variety of adapters and accessories for any solvent or seal wash bottle
- Significantly reduces exposure to organic vapors



What we need to know before making a recommendation for MAC-MOD SafetyCaps?

1. How many bottles need a MAC-MOD SafetyCap?
2. How many tubes (holes for each cap) are needed for each bottle?
3. What exact OD (outer diameter) do the various tubes have?
4. What thread size do the bottles have?



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The MAC-MOD SafetyWasteCap System

Status Quo



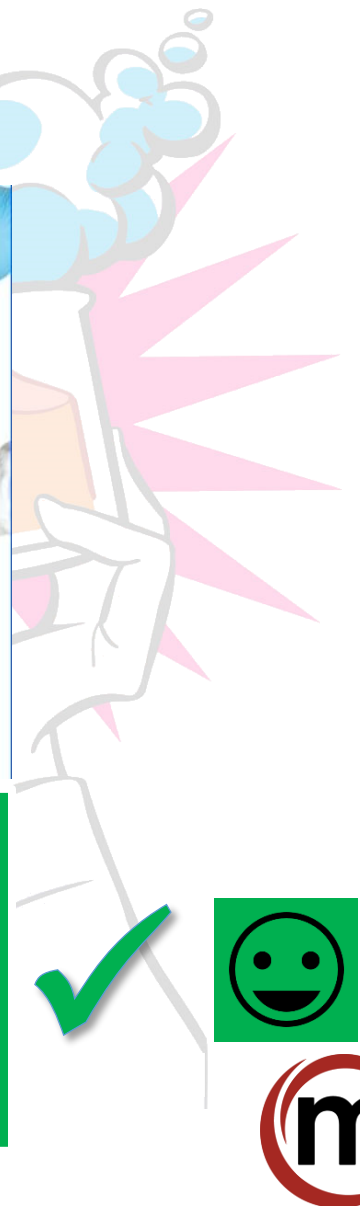
- Harmful vapor emission
- Safety issue for employees
- Possible fire hazard
- Danger of overfilling
- Violation of safety regulations
- Fails safety inspections



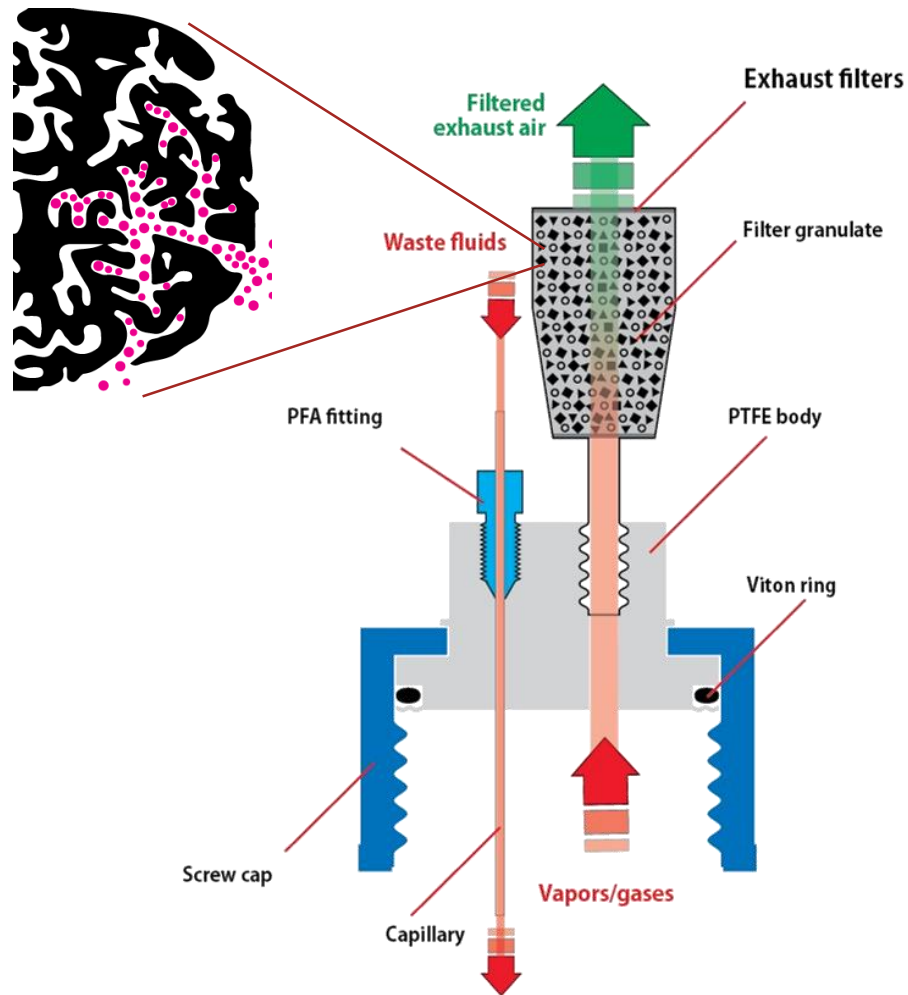
MAC-MOD SafetyWasteCaps



- Hermetically sealed → no harmful vapors
- Easy container change
- No tubing slippage
- Different thread sizes
- Passes the safety inspections



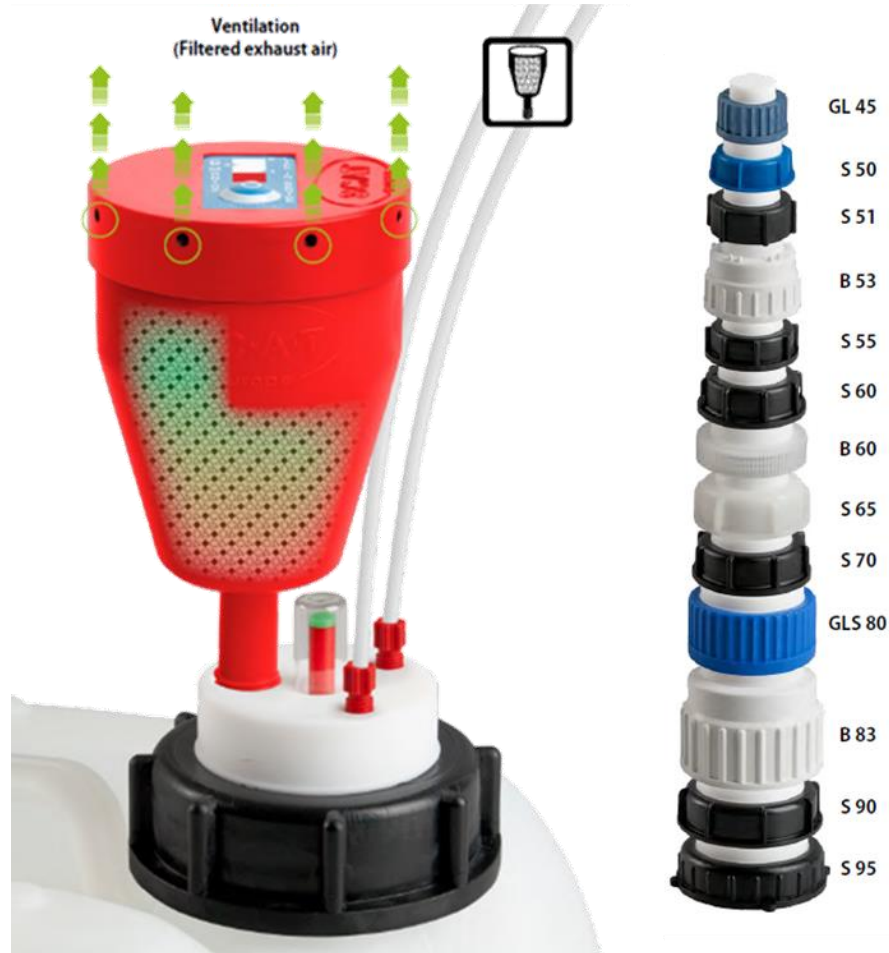
Dynamics of the Waste Cap



- Waste containers receive and contain different waste solvents and chemicals.
- The exhaust filter contains a special multicomponent granular mixture of highly activated carbon.
 - Optimum filter media for solvent vapors
 - Specific filtering surface of 1,200 m²/gram
 - Contains components that prevent clumping of the activated carbon and ensure maximum filter performance



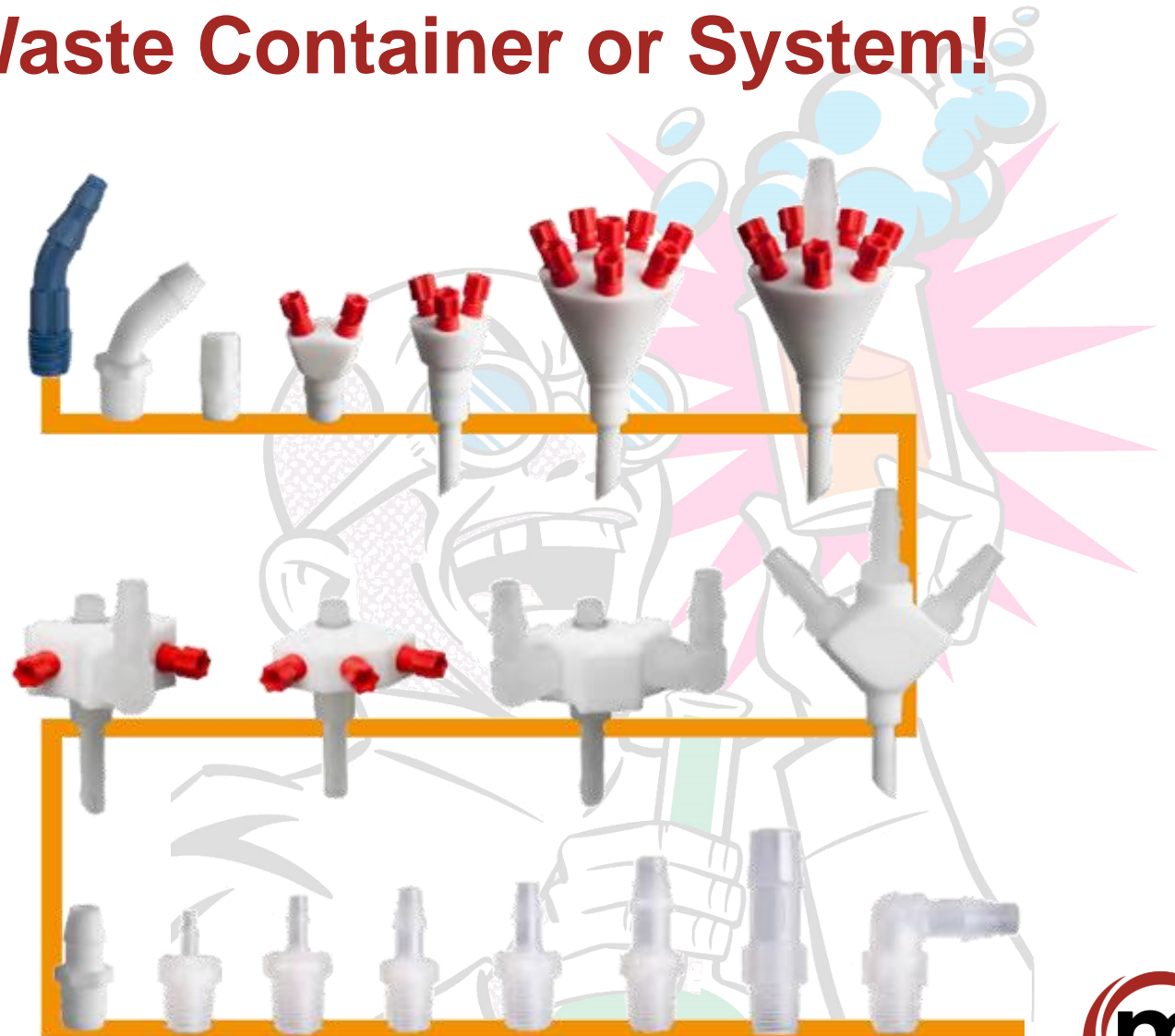
MAC-MOD SafetyWasteCaps



- SafetyWasteCaps are available for a wide range of **different container threads**.
- The exhaust filter equalizes the pressure in both directions (inward and outward) to avoid underpressure or overpressure inside the container.



Adaptable to Suit Any Waste Container or System!



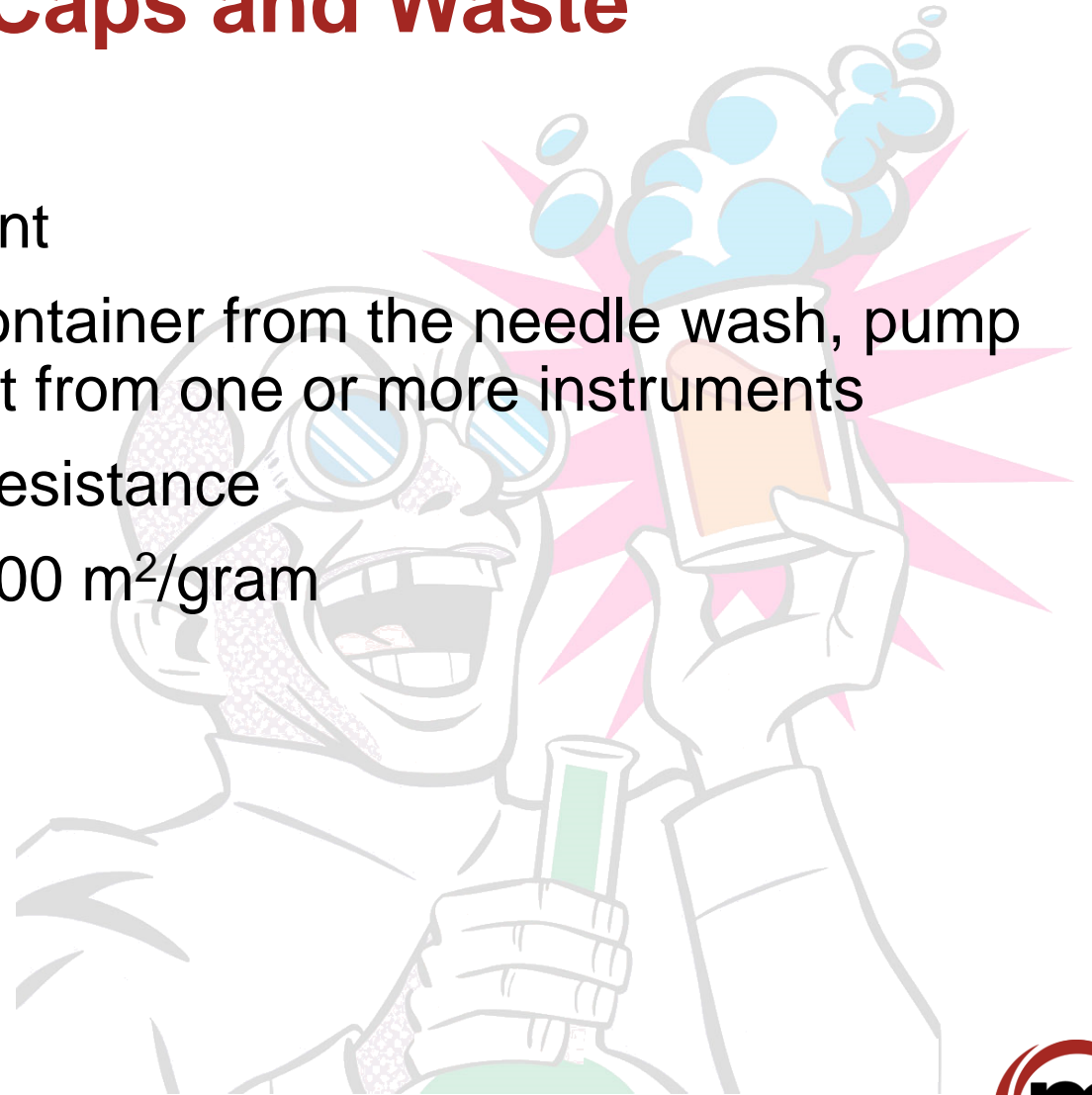
What we need to know before making a recommendation for the SafetyWasteCaps and Containers?

1. How many tubes (holes per cap) per bottle are needed for your MAC-MOD SafetyWasteCap?
2. What exact OD (outer diameter) do the tubes have coming from your instrument(s)?
3. Do you want to retrofit your current container OR do you want to purchase a new solution?
4. What thread size do the waste containers have?



Advantages of SafetyWasteCaps and Waste Containers

- Protect your health and lab environment
- Multiple connections to same waste container from the needle wash, pump seal wash, purge valve and LC effluent from one or more instruments
- Best available materials for chemical resistance
- Activated carbon filter surface area 1200 m²/gram



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Case Study I: Independent Study Performed by SGS Fresenius Institute

- Current Status Quo Solvent Reservoir Arrangement for many HPLCs and UHPLCs across the country



- SGS Fresenius Institute designed an independent study to demonstrate the solvent losses with the “Status Quo” situation vs. the MAC-MOD SafetyCaps Solution
- Measurement of **loss of organic modifier** for four different caps
 - MM Safety cap
 - Solid cap (no hole)
 - 1-holed cap
 - 3-holed cap
- **Changes in chromatograms** for isocratic separation (premixed mobile phase) of 3 PAHs (Polycyclic Aromatic Hydrocarbons) over a 31-day period.



Test Conditions and Instrument Setup



Bottle A: This bottle was closed using a MAC-MOD SafetyCap with a GL45 Thread



Bottle B: This bottle was tightly closed with its standard GL45 cap, which includes PTFE film disk for sealing



Bottle C: This bottle was closed using a cap with a 10 mm hole in the plastic material, yielding an open exit area of $\sim 0.785 \text{ cm}^2$

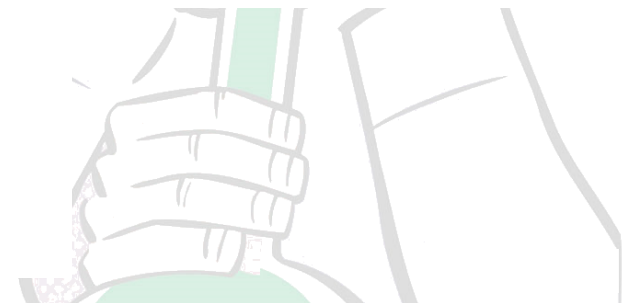


Bottle D: This bottle was closed using a cap with three 3-mm holes in the plastic material, yielding an open exit area of $\sim 0.212 \text{ cm}^2$



HPLC System:

- Hitachi LaChrom Elite® system with Diode Array Detector
- Isocratic pump conditions and premixed mobile phase
- **Mobile Phase: 80:20 (v/v) methanol/water, premixed**
- HPLC Column: C18, 5 micron, 4.0 x 125 mm



Weight changes due to solvent loss after 31 Days:

SafetyCap



Sealed



1-Hole



3-Hole

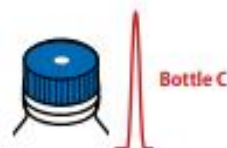


	Bottle A	Bottle B	Bottle C	Bottle D
Day 1	457.45	539.26	724.14	715.08
Day 31	457.43	539.26	672.45	687.36
Loss (g)	0.02	0.00	51.69	27.72
Loss (%)	0.0	0.0	7.14	3.88

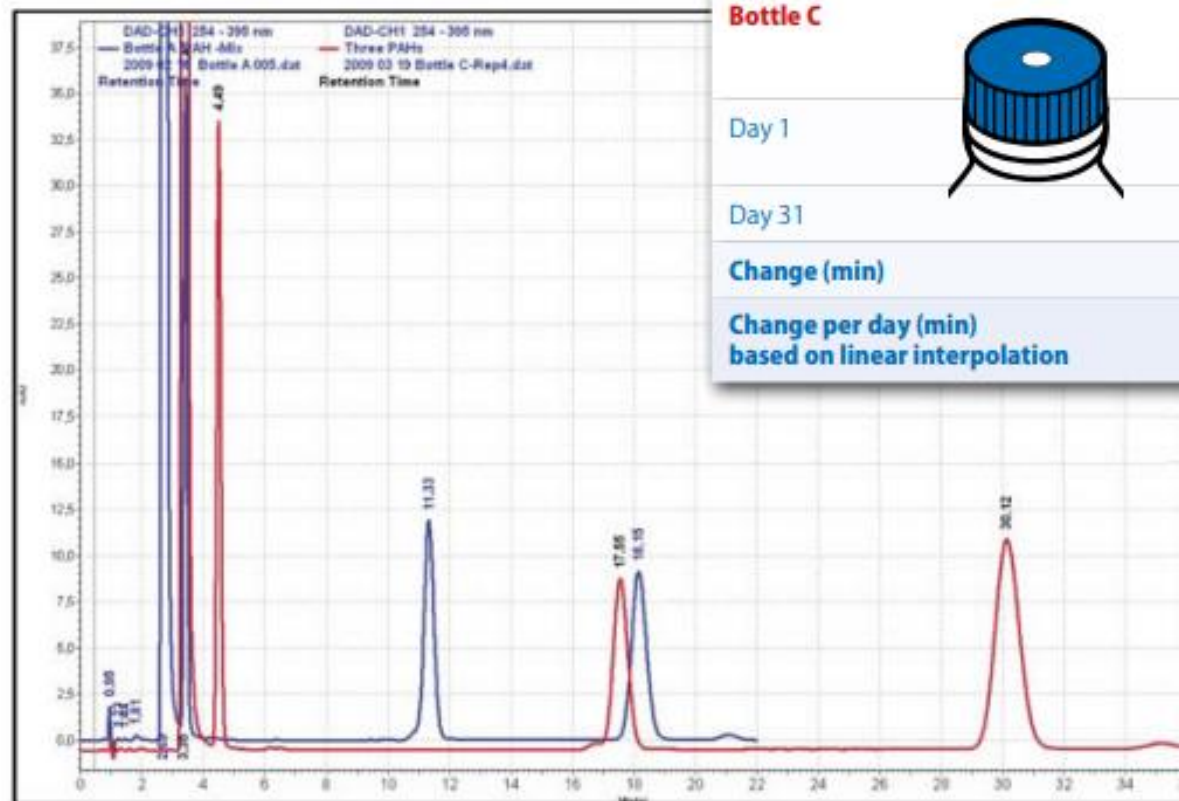
Methanol weight loss for Bottle A (Safety Cap) was negligible (.02 g total loss!!)



Retention Time Changes from separations using solvent Bottle C



With S.C.A.T. SafetyCap closed bottle and **bottle C**



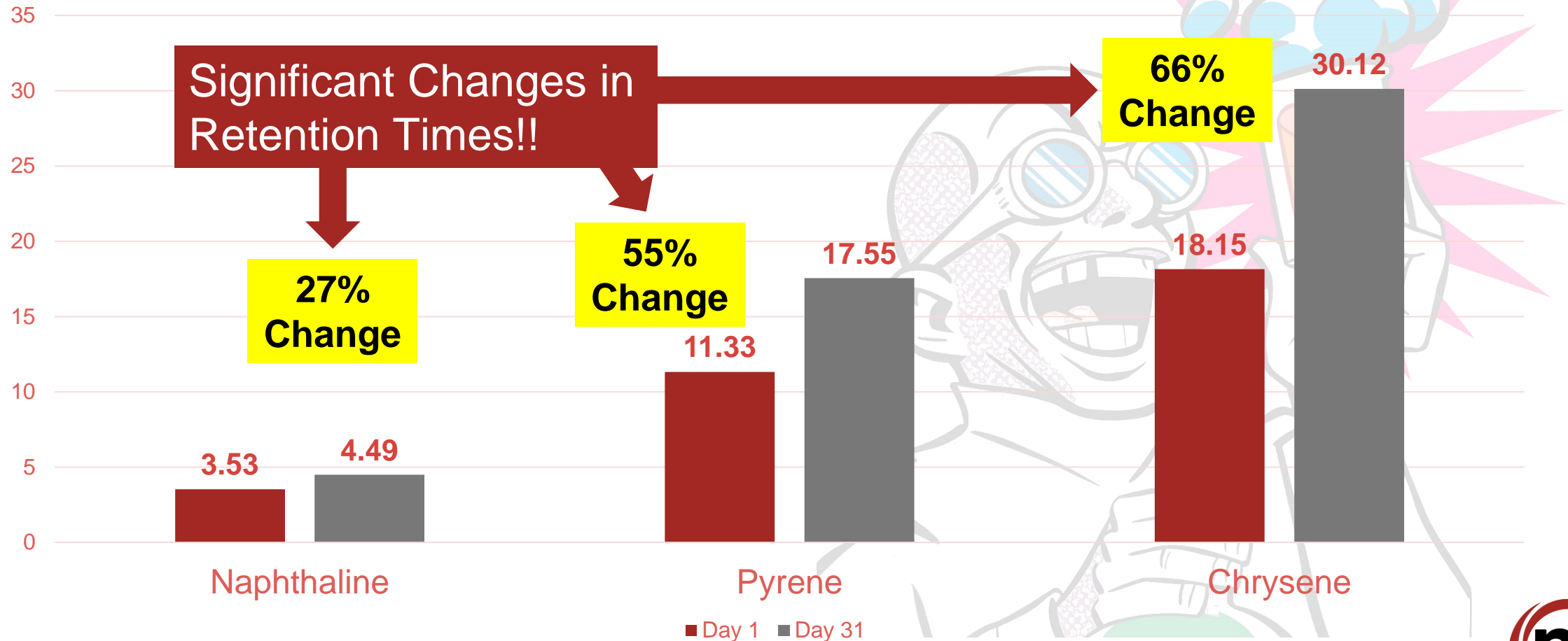
Bottle C



Retention time changes

	Napthaline	Pyrene	Chrysene
Day 1	3.53	11.33	18.15
Day 31	4.49	17.55	30.12
Change (min)	0.96	6.22	11.97
Change per day (min) based on linear interpolation	0.031	0.201	0.386

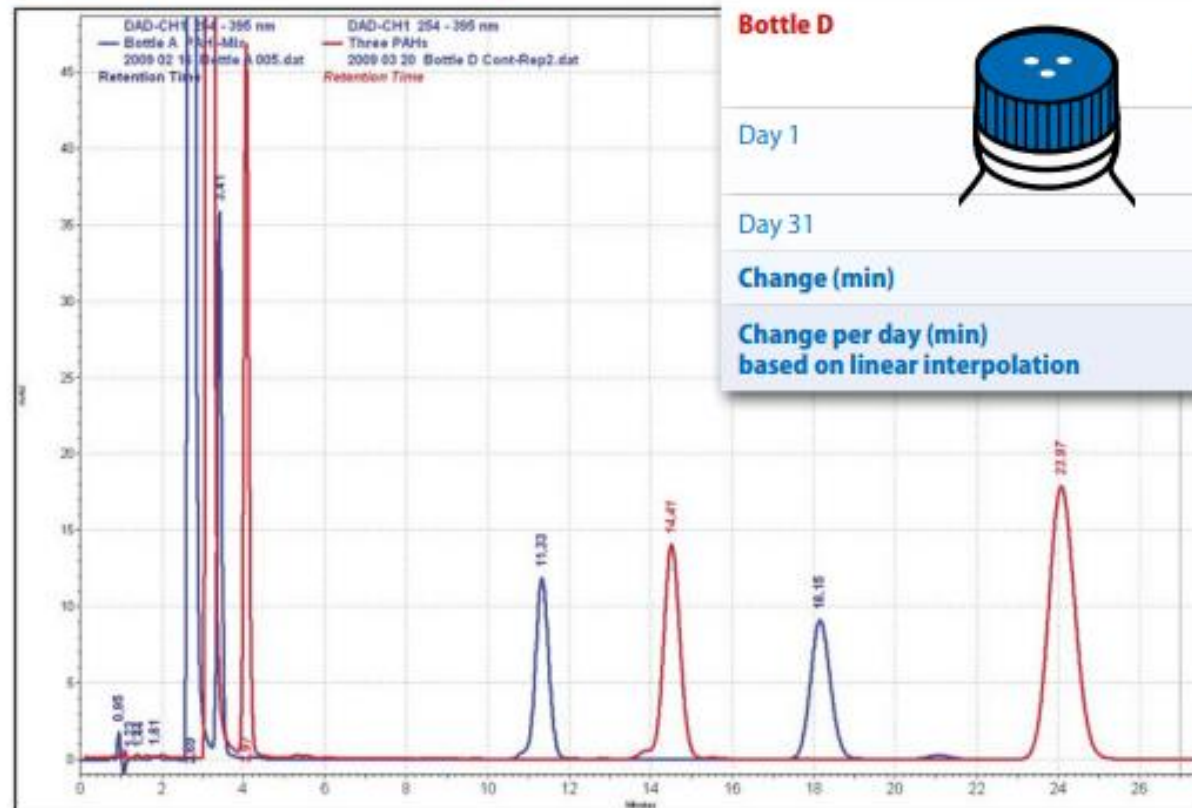
Graphical Representation of Retention Time Changes for Bottle C (one 10 mm diameter drilled hole)



Retention Time Changes from separations using solvent Bottle D



With S.C.A.T. SafetyCap closed bottle and **bottle D**



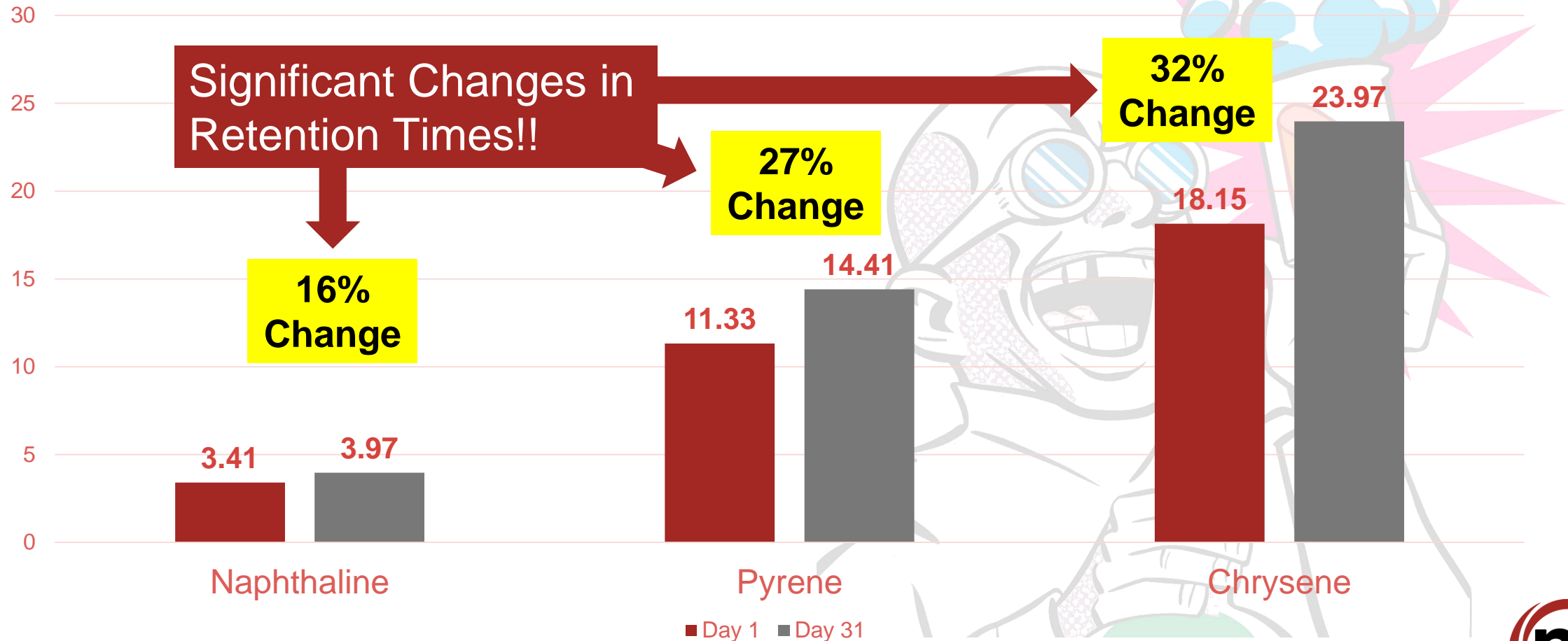
Bottle D



Retention time changes

	Napthaline	Pyrene	Chrysene
Day 1	3.41	11.33	18.15
Day 31	3.97	14.41	23.97
Change (min)	0.56	3.08	5.82
Change per day (min) based on linear interpolation	0.018	0.099	0.188

Graphical Representation of Retention Time Changes for Bottle D (3 drilled holes of 3 mm diameter each)



CH₃CN and CH₃OH Emissions from Bottle with No Cap vs. Bottle with SafetyCap in test chamber with air exchange

In order to investigate the atmospheric emissions caused by open solvent bottles in comparison to a solvent bottle with S.C.A.T. SafetyCap, one of each solvent bottle was placed in a test chamber, and their respective methanol or acetonitrile emissions were tested after 1, 3 and 7 days



Concentration ratio of ~150:1 (mg/m³)

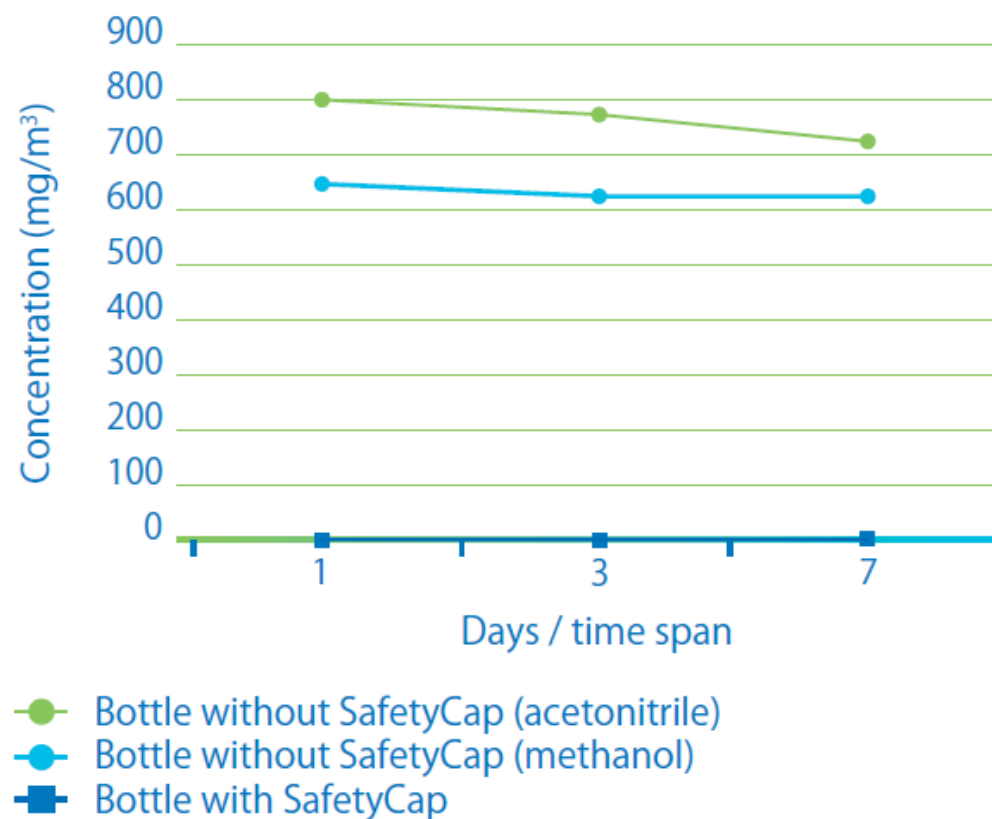
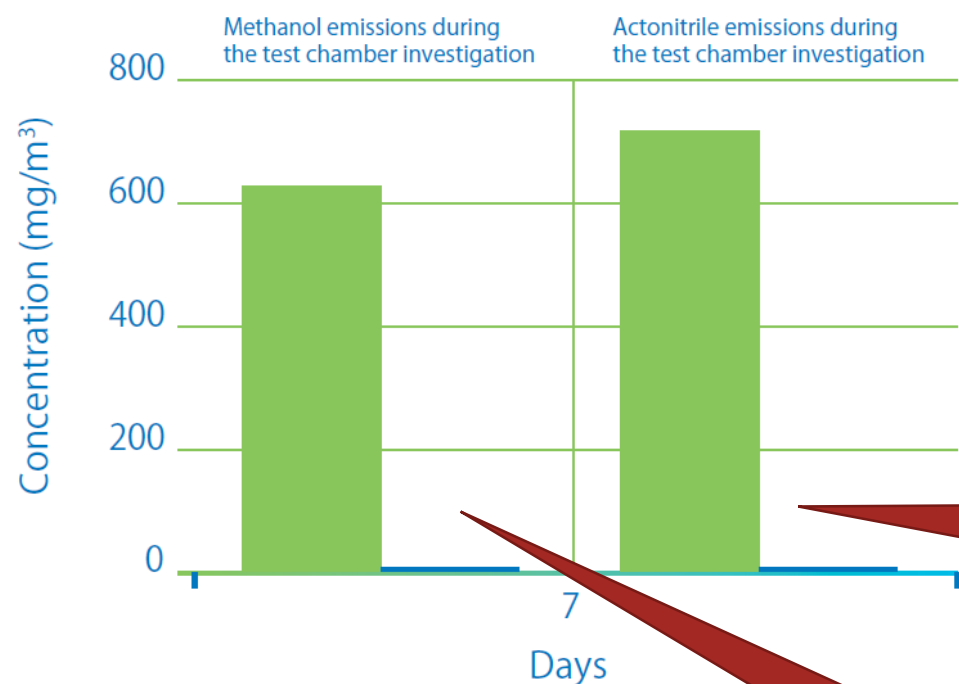


FIGURE 3. Methanol and acetonitrile emissions in the test chamber.

CH₃CN and CH₃OH Emissions from Bottle with No Cap vs. Bottle with SafetyCap in test chamber with air exchange



Within the test chamber, **despite continuous air exchange**, a methanol concentration of **630 to 660 mg/m³** was found in the chamber for the solvent bottle **without the SafetyCap**, whereas a methanol concentration of **1 to 2 mg/m³** was for a solvent bottle **with the SafetyCap**.

Similar results were obtained for acetonitrile (**730 to 800 mg/m³** for solvent bottle **with no cap** vs. **1 to 5 mg/m³** **with the SafetyCap**).

>17 mg/m³
Considered
Dangerous!!!

>270 mg/m³
Considered
Dangerous!!!

- Methanol emissions without SafetyCap
- Methanol emissions with SafetyCap
- Acetonitrile emissions without SafetyCap
- Acetonitrile emissions with SafetyCap



Case Study II: Fitting the “Unfittable” Container

The Status Quo at Customer Site:



- Analyst approached us about a customized solution
- **These 1-gallon reservoirs are used in all labs across multiple sites because they are compatible with the incinerator**
- They could not change their current waste reservoir
- Current solution was not sufficient to keep harmful vapors from escaping into the lab



MAC-MOD SafetyWasteCaps Customized Solution



MAC-MOD SafetyWasteCaps

- Customized lid for 1-gallon jugs
- Multiple ports for Tygon tubing with feeds from LCs and purge valves
- Activated carbon solvent filter with change indicator shows elapsed service life clearly

A Better Solution!



Standard
secondary
container



Largest Solvent Safety Product Range Worldwide



SafetyCaps

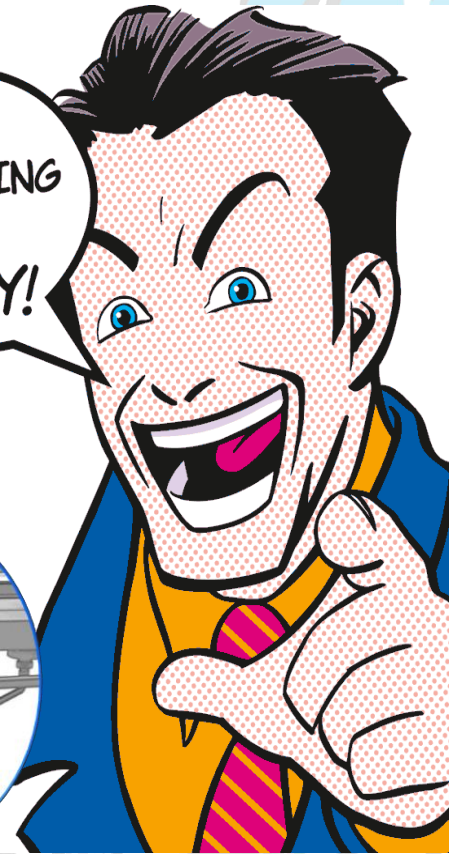


WasteCaps



Safety Funnels

OWN
MANUFACTURING
MADE IN
GERMANY!



Level Control



Safety Containers



Accessories



Built-In Solutions



Additional accessories for SafetyCaps and SafetyWasteCaps

“The Werner” for purging



**CLEAN AIR.
CLEAN HPLC.**

Part No. 106 660

**Purging manifold
The „Werner“**

- GLS 80 (f) thread
- 4x GL 45 (m) connections
- Electrostatic conductive PE-HD



Part No. 107 910

SafetyCap III GL 45

- incl. 3x Fittings for capillaries with 3.2 mm Ø outer diameter
- incl. air valve with filter function



Part No. 501 151

DURAN® laboratory bottle with wide neck opening

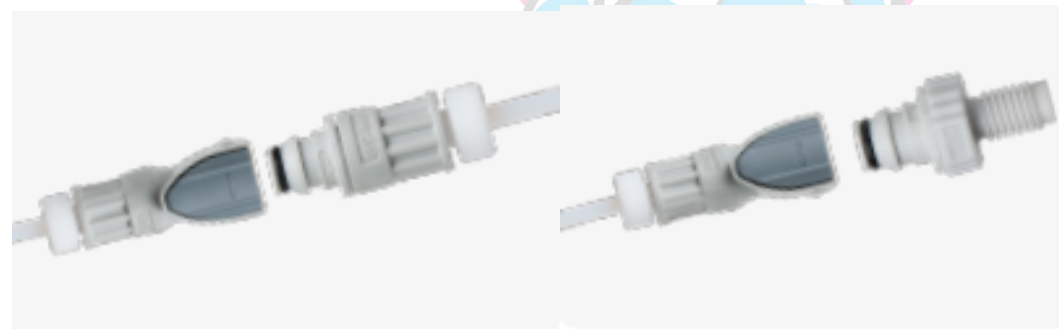
- GLS 80
- 1,000 ml
- Clear glass
- Round

More containers and laboratory glass bottles:
www.scateurope.com



Simply close unused connections with standard bottle closures.

CPC Quick Disconnect Couplings



Funnels for Solvent or Waste Addition



Containers – Bottles, Canisters, Politainers, Collecting Trays

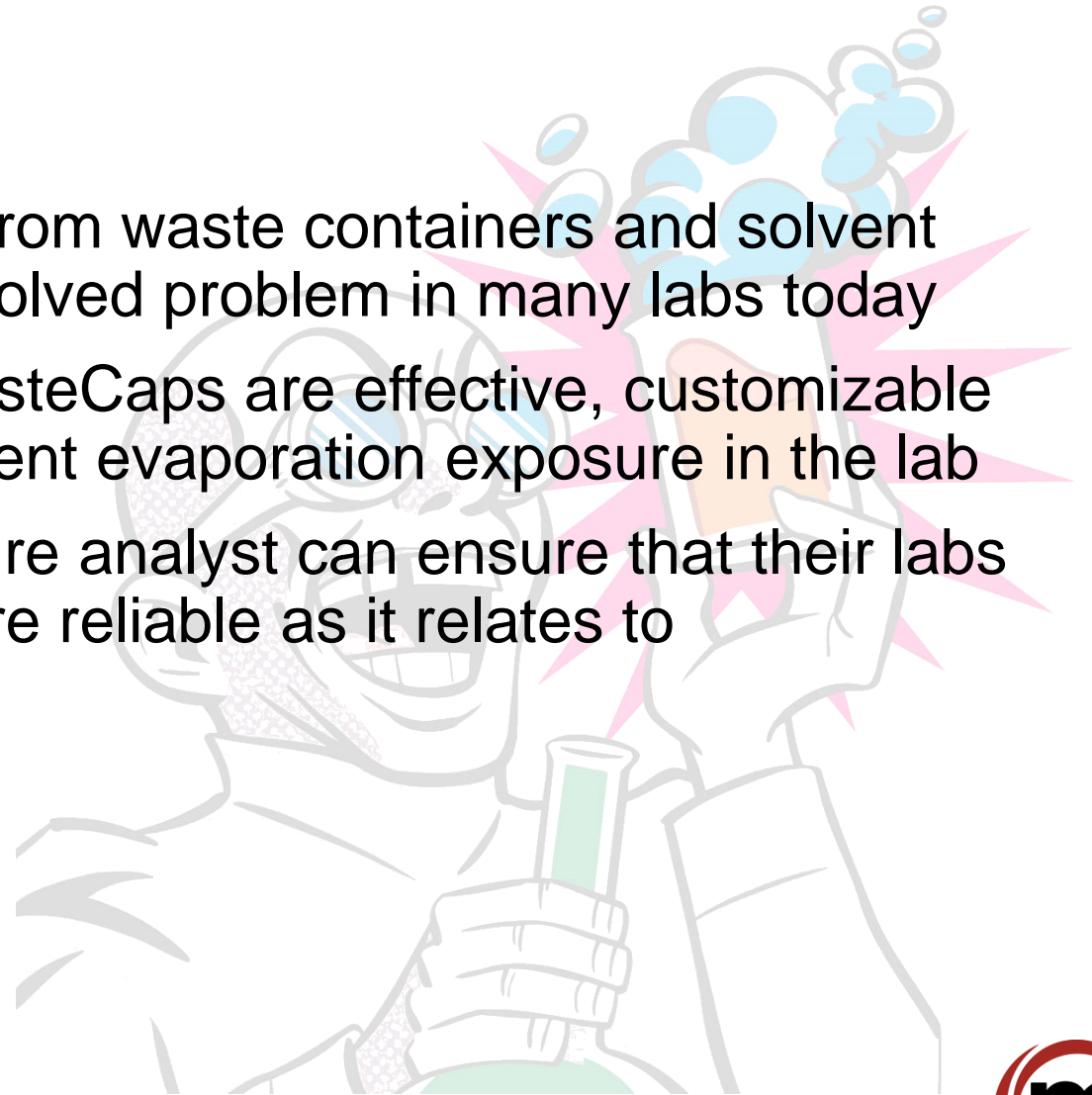


- All **Bottles and Canisters** are suitable with all SafetyWasteCaps.
- **Canisters** with UN approval are permitted for transport of hazardous goods on roads and plant premises.
- Canisters in black are made of electrostatic conductive PE-HD.
- Fluorinated canisters protect against weight loss of content. Fluorination on both sides protect the canisters plastic walls from permeation of chemicals.
- Level control integrated floater for an optical level control.
- **Politainer** can ideally be stored space-saving prior to filling and it is stackable when filled.
- **Collecting trays** with base insert, the waste canisters always stay dry.



Conclusion

- Solvent evaporation in the laboratory from waste containers and solvent reservoirs is a major issue and an unsolved problem in many labs today
- MAC-MOD SafetyCaps and SafetyWasteCaps are effective, customizable and versatile solutions for limiting solvent evaporation exposure in the lab
- By limiting solvent evaporation exposure analyst can ensure that their labs are safer, more cost effective, and more reliable as it relates to chromatography.





Thank You For Your Time