Universal PFAS restriction proposal - Public consultation contribution on laboratory water systems

This contribution to the public consultation on the universal PFAS restriction proposal focuses on two different aspects in providing pure and ultrapure water.

1. Use of PTFE (Polytetrafluoroethylene) coated, FKM (Fluorine Rubber) and FFKM (Perfluoroelastomer) gaskets to avoid water contamination due to leaching from sealings (O-rings and diaphragms) and high resistance to UV irradiation.
2. Use of PTFE as a reactor block in the ultraviolet (UVC) light treatment of lab water to inactivate microorganisms.

Laboratory water

Ultrapure water is water that has been purified to an extremely high degree, typically through multiple complex purification processes. This level of purity offers critical benefits for scientists. With our Milli-Q® water systems we have been able to provide ultrapure water free of substances of concern and other contaminants such as PFAS, pesticides, phthalates, endocrine disruptors, etc.

Many fields of scientific applications where even the slightest presence of impurities in the water will lead to false results or may interfere with the target compounds require ultrapure water. The non-exhaustive list below gives some examples:

- Cell Culture and Biotechnology: Cell culture work, especially in biotechnology and cell biology, requires ultrapure water to maintain the health of cells and prevent any potential contamination. Even low levels of contaminants in water can affect cell growth and behavior.
- Microelectronics and Semiconductor Manufacturing: In the semiconductor industry, ultrapure water is used extensively for cleaning, rinsing, and etching processes. Any impurities can cause defects in microelectronic components.
- Life Science applications: Molecular biology applications, e.g., PCR and DNA sequencing
- Environmental Analysis: Environmental scientists use ultrapure water to prepare samples and standards for water quality testing. Contaminants in the water being tested can lead to inaccurate assessments of environmental conditions.
- **Sensitive Analytical Techniques:** Scientists using sensitive analytical instruments like high-performance liquid chromatography (HPLC), mass spectrometry (MS), or atomic absorption spectroscopy (AAS) rely on ultrapure water as a solvent or reagent. **Any**

impurities in the water could lead to inaccurate readings or damage to the equipment. In case scientists want to measure PFAS in an environmental sample, PFAS must not be introduced via ultrapure water. Otherwise, the researchers cannot discriminate whether measured PFAS was in the sample or in the water used to prepare the sample.

Usually, a combination of advanced technologies is involved in purification stages including ion-exchange resins, cleaner activated carbons, etc.

The implementation of the current universal PFAS restriction proposal would end the supply of ultrapure water for laboratories. Fluoropolymers, fluororubbers and perfluoroelastomers are in the scope of the restriction and are not derogated for their specific use in laboratory water systems. Hence, 18 months after entry into force, we would be forbidden to provide the Milli-Q® IQ 7000 series and we also could not provide several consumables for Milli-Q® and other laboratory water systems. Also, spare parts would become unavailable.

Though we are constantly working on the further improvement of our high-quality equipment, the removal of fluoropolymers, fluoroelastomers and perfluoroelastomers from the systems cannot immediately be compensated by other materials. To date materials with similar properties (low leaching, stable to UV irradiation and pure water over several years) as a drop-in alternative are not available.

With 44 patents with a focus on sustainability and contaminant removal in laboratory water solutions and a global market share of 50 % in 2022[1], Merck Life Science is a key player in the laboratory water business and a major provider of all product types through products like the new Milli-Q® IQ 7000 water purification system. With our headquarters located in Darmstadt, Germany we are committed to the goals of the European Union to help improve the well-being of its citizens and a healthy environment.

What are the different laboratory water grades?

Water grades in the lab are defined by quality standards, such as the ASTM D1193 or ISO 3696, which help to ensure that the correct water quality is used for specific applications. Milli-Q® IQ 7000 series systems provide ultrapure water that even exceeds the definition for water type 1 since for special applications like trace metal analysis, ultrapure water quality must go beyond type 1 specifications.

Why is the type of water relevant in the context of the PFAS restriction proposal and a possible ban of fluoropolymers and perfluoroelastomers?

Both polymers are chemically inert and do not release significant levels of chemicals/contaminants into the ultrapure water. With other materials available to date and

[1] SDi Global Assessment Report 2023 – The Laboratory Analytical and Life Science Instrumentation Industry

to us, contamination reaches an unacceptable grade and hence negatively interferes with research and innovation.

With appropriate material selection and embedded technologies, ultrapure water is suitable for the most stringent trace elemental analyses since trace contaminants and microorganisms are eliminated.

The Milli-Q® IQ laboratory water series

Our Milli-Q® water systems are an overly complex combination of technologies compiling more than 500 raw materials. A maximum of 1 % of those raw materials contain or are PFAS and are required (as of today) to deliver the ultrapure water needed by scientists.

We have demonstrated through scientific analysis (certified by external testing labs) that our solutions:

- Do not leach any PFAS from any raw material in the ultrapure water and
- In the case that customers' tap water contains PFAS, we could demonstrate that our filtration solutions remove all traces of PFAS from the ultrapure water.

Our lab water purification portfolio includes pure (Type 2 and reverse osmosis water), and ultrapure (Type 1 and even exceeding Type 1 requirements) laboratory water systems designed for scientists in validated and non-validated environments. These include pharmaceutical, clinical, academic, industrial, research, and government laboratories. Milli-Q® systems produce high-quality purified water as an essential raw material to reliably support specific applications, to feed equipment and instruments, and for general laboratory use.

With its Milli-Q® IQ 7000 series Merck Life Science KGaA offers a wide range of water purification systems that are produced in the EU.

The Milli-Q® systems have always been developed taking into consideration 2 key elements:

- Ensure to provide the most appropriate quality of water to our customers,
- Always integrate the latest technologies/solutions to deliver the best standard from a sustainability point of view. As an example, Milli-Q® IQ 7000 series from Merck is the first lab water solutions being mercury free.

Laboratories are often equipped with water purification systems, such Milli-Q® systems, to produce both types of water: pure and ultrapure water. Milli-Q® systems are built with different modules depending on the level of desired water quality.

To achieve and maintain this high performance, regular monitoring and maintenance of these systems are necessary to ensure consistent water quality and reliable experimental outcomes.
Additionally, depending on the regulatory environment, the water quality might have to meet or exceed and be compliant with norms and standards.

To be able to provide lab water of such a high quality a couple of requirements are met by the Milli-Q® IQ 7000 series:

- Feed water (generally tap water) needs to be purified (freed from chemicals and biological contaminants). To achieve this, the system uses several purification media in cartridges like the IPAK Gard (pleated filter, carbon), a reverse osmosis cartridge followed by an Elix® electrodeionization module.
- The purified water is further directed through a UVC light reactor to inactivate microorganisms that may still be present in the water. The mercury-free ech$_2$o® bactericidal UVC LED works in a reactor made of PTFE (see below for more details).
- After this step, the water is directed to a storage tank where the quality of the water is maintained by an Automatic Sanitization Module (ASM) that also uses a mercury free ech$_2$o® UVC LED to prevent the formation of biofilms (see Figure 2).
- From the storage tank pure water (type 2) can be used via an E-POD® pure water dispenser or can feed a polishing Milli-Q ® equipment.

Thus, we contribute to our customers efforts towards a higher degree of sustainability by phasing out mercury. Currently, this is not possible without using PTFE. Due to the lower energy consumption, the UV radiation wavelength, and the design of the UV source (single UV LED vs long UV lamp), the UVC LED alone is not equivalent to the mercury-based UV lamp. Therefore, a highly reflective reactor is needed to achieve similar results compared to the combination of stainless steel and a mercury lamp. We are using a reactor that is made entirely of PTFE (not applied as a coating to another material), since this has proven to be the material with the highest reflectivity to ensure the optimized use of energy emitted from the UV LED through the entire photooxidation reactor.

Where ultrapure water is needed the water is treated with a Xenon excimer oxidation UV lamp (also mercury-free but not using a PTFE reactor) emitting at 172 nm for photooxidation of organic contaminants. To date, we are the only supplier offering a total mercury-free (ultra)pure water purification device. To ensure leak proof mounting of the UV lamp quartz housing, two FKM O-rings are used as these materials need to resist UVC irradiation (Figure 1).

Figure 1: UV lamp quartz housing with FKM O-rings

Water is further sent through an IPAK Quanta® polishing cartridge to remove ions and organic contaminants. After polishing, the water can be delivered via the Q-POD® ultrapure water dispenser or it is recirculated to the storage tank.

All these purification cartridge/packs and UV lamps are consumables and need to be replaced after their recommended service life.

For a proper and durable sealing, to avoid the introduction of contamination, the consumables are fitted with O-rings that are made of fluoro- and perfluoroelastomers (PTFE coated NBR, FKM or FFKM), which have low leaching of chemicals also under mechanical pressure.

Where parts of the equipment are connected to each other, diaphragms, also made from perfluoroelastomers, are used for the same purpose; very low leaching under mechanical stress.

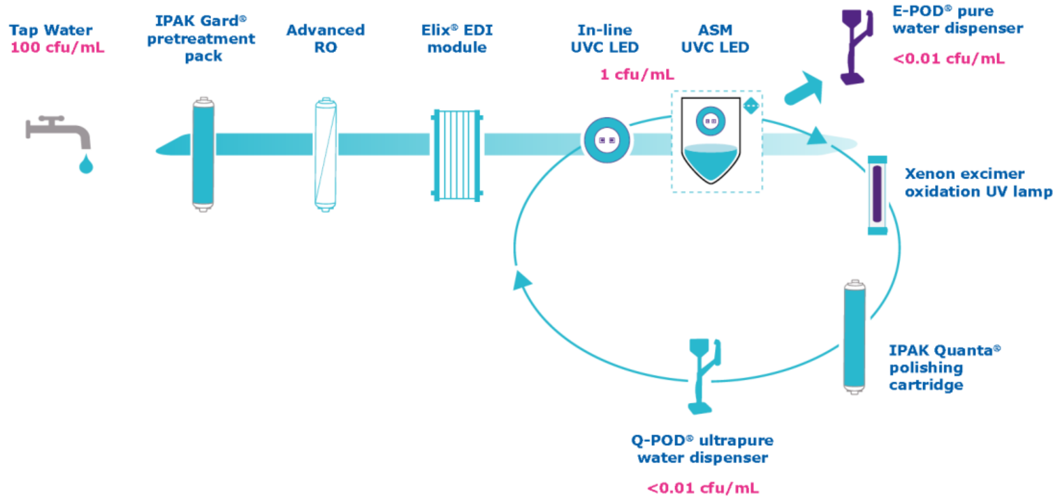

Figure 2: Preparation and supply of ultrapure water. Tap water flows thru a set of cleaning modules (IPAK Gard®, Reverse Osmosis (advanced RO), Elix® EDI module), and microorganisms are removed using UVC light. It is kept in the storage compartment at the level of quality with UV light. The pure water is then purified further through excimer UV lamp (organic removal) and a polishing module (IPAK Quanta®). The connection of all these parts requires low leaching sealings.

Using ultrapure water from a Milli-Q® IQ 7000 series system, the Milli-Q® IQ POD Element purifies further to deliver ultrapure water for trace elemental sensitive applications. The water dispensed at the point of use is confirmed to contain extremely low levels of elemental contaminants, from single ppt to sub-ppt detection levels.
Independent laboratories specialized in ultra-trace elemental analyses have verified the unit's water quality.

Sealings (O-rings, gaskets and diaphragms)

Laboratory water systems are made from numerous components (tubes, valves, reactors, sealings etc., see overview in Figure 2). Some of these components are made from smaller articles themselves (like valves). All components and sub-components need to be made of materials that have a very low leaching potential and hence do not release significant amounts of chemicals/contaminants into the lab water. Whereas this can be achieved for a couple of plastics parts that mainly serve as flow-through parts in the system, filters and sealings are constantly under mechanical stress while the system is in operation. Therefore, the requirement for low leaching materials in these parts is even more important compared to the other components.
During the development of our current lab water systems, different O-rings and diaphragms made of different materials were tested as sealings about leaching.

We present measured values for the leaching of EPDM, NBR, FKM and FFKM in the confidential attachment.

The data provide evidence that diaphragms and O-rings made from perfluoroelastomers are the best available material to ensure delivery of highest purity water from benchtop systems.

EPDM O-rings can also be found in water purification systems in the connection between consumables and systems. However, they are used in the very early steps of the purification process and hence leaching molecules are eliminated in the further course of the purification. When the water has reached a certain degree of purity, the reintroduction of chemicals via leaching must be at a minimum. To date this can only be achieved using the FKM O-rings.

There are also older water purification systems in operation in laboratories all over the world which still rely on the use of mercury lamps. Gaskets, diaphragms and sealing used in these systems and exposed to the high energy UV light as generated by the mercury lamp can only withstand that radiation when made from FKM or FFKM. Hence, also the supply of spare parts made of FKM and FFKM needs to be secured within a derogation. It is not possible to re-validate a system in operation.

For consumables laboratories may dispose the consumable as laboratory waste and we can also take them back.

For the use of FKM and FFKM used in different parts of the Milli-Q® IQ 7000 series and spare parts for older systems that are in operation, we ask for a derogation of 12 years for these uses combined with a review by the Commission after 7 to 8 years regarding the proceedings on the development of alternative materials and technologies.

PTFE use as reactor block in UVC-light treatment

Pure and ultrapure water not only needs to be free of chemical contamination, it also must be free of microorganisms like bacteria. While this is achieved during the initial preparation by the purification modules (especially by advanced reverse osmosis, removal of 95 to 99 %), in the further preparation of the lab water, the remaining bacteria need to be blocked from proliferation. This is generally achieved by using UVC light at a specific wavelength in different stages of the water preparation.

Which wavelength inactivates bacteria best?

To disable bacterial replication, DNA and RNA are strategically targeted with the use of radiation. Figure 3 shows the absorbance spectra of the four nucleotides in DNA. The absorbance maximum of DNA is assumed to be between 260 and 270 nm. The optimal wavelength to disable microorganisms and viruses is around 265 nm.

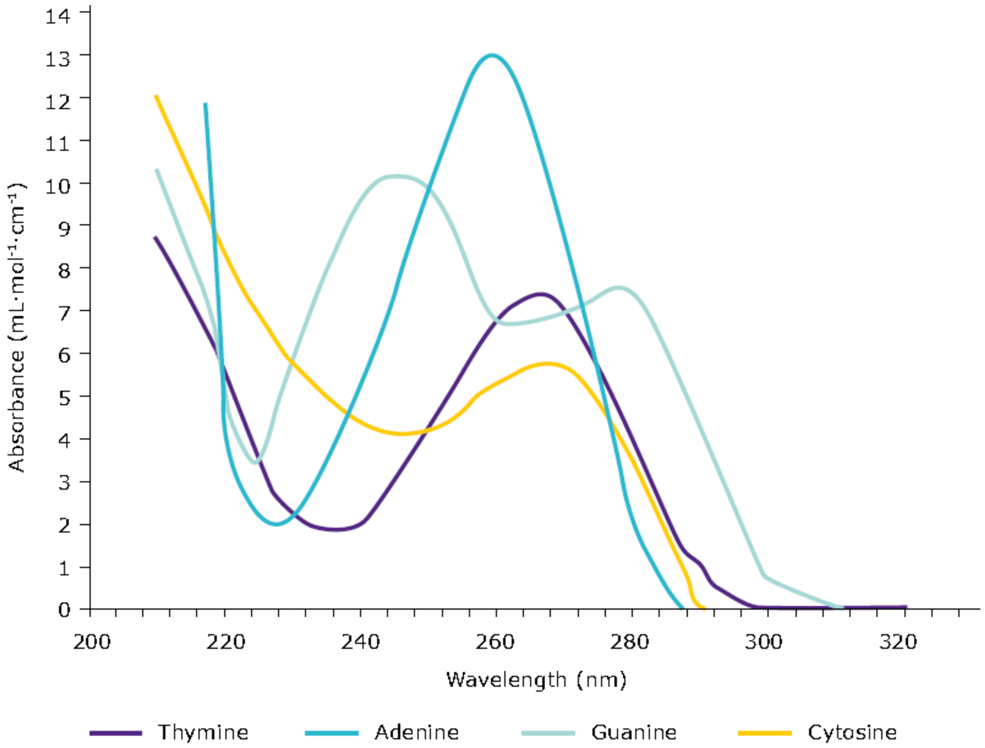

Figure 3: Absorbance spectra of DNA nucleotides

Lab water systems need to provide a very high degree of purity by on the one hand removing particles, chemicals and biological material from the feed stream, which commonly is potable water. On the other hand, chemicals must not be released by the system itself, e.g. leaching from sealings.

Particles may be removed by filters with a defined pore size. Bacteria are also removed by reverse osmosis and can be inactivated by UV light.

In benchtop lab water systems advanced reverse osmosis clears water of 95 to 99 % of the bacteria, and the concentration is further reduced by UVC light. Merck Life Science KGaA was able to replace the mercury containing light source formerly used together with a stainless-steel reactor with an UVC diode that allows a compacter design of the system and reduces the energy needed to generate the UVC light. However, lower UVC power output and high operating temperatures are weaknesses of this UVC source.

The UVC dose is a function of UVC irradiance and exposure time. Therefore, the UVC light needs to be reflected in the reactor to achieve the same amount of efficiency compared to a mercurylamp-based system.

Though very costly, the material that turned out as the best available solution is a reactor made from PTFE (Figure 4) because it best reflects UVC light and thus enhances exposure time. It was demonstrated that the reflectance of PTFE in liquids are between 76 and 90 %[2].

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[2] https://www-eng.lbl.gov/~shuman/NEXT/MATERIALS%26COMPONENTS/MISC/PTFE-Reflectance-ThesisCoimbra.pdf

Figure 4: PTFE reactor for UVC light treatment of lab water

UVC LEDs are constantly optimized for higher energy output and efficiency. Further, different technologies, for example the use of lenses to better distribute UVC light in a reactor, are under development and Merck Life Science KGaA closely follows these developments and investigates their applicability in its laboratory water systems. To date, these potential alternative solutions are not feasible and cannot replace the PTFE reactor.

Merck Life Science KGaA is constantly working on developing new products and also to improve the existing portfolio. With the Milli-Q® IQ 7000 series we have brought a unique system to the market. It is capable to produce ultrapure water directly from tap water, offers the highest currently technical possible water purity and does not anymore rely on the use of mercury lamps for the control of bacterial growth and the generation of biofilms in the system.

The systems so far used by laboratories and QA institutions are far from the end of their service life. At the end of the service life, systems are taken back by Merck Life Science KGaA because they are electrical equipment and as such subject to directive 2012/19/EU.

Based on these considerations Merck Life Science KGaA will follow the following approach: Development of new laboratory water systems will consider the technological progress that may in the future also replace the UVC LED-PTFE reactor system with alternative materials. The energy output of UVC LEDs is an ongoing research topic and in time the need for the very high reflectivity of PTFE may not be required anymore. Changes to the system also requires a new development of the whole UVC-LED-reactor part since water needs to remain in the reactor long enough to achieve an acceptable degree of bacteria deactivation. Therefore, the development of a new systems is not a simple discovery of a material with a reflectivity comparable to PTFE and the identical robustness of PTFE. It rather is a complete re-design of the bactericidal treatment module system, that also requires extension validation.

As mentioned above, benchtop lab water systems, besides the consumables, have an envisaged service life of at least a decade. For a sustainable shift towards alternative technological feasible solutions, we require a 12-year derogation with the option for a review after 7 to 8 years by the Commission for the use of PTFE as reactor material from the universal PFAS restriction for

1. the development of feasible alternatives to the combination of UVC LED and PTFE reactor without falling back to mercury lamps
2. ensuring the continuing availability of pure and ultrapure water as an essential raw material for the science and research community
3. ensuring the availability of ultrapure water as a reference material

Conclusion

The universal PFAS restriction must not result in a lack of ultrapure water in laboratories. This would make environmental monitoring for contaminants of all types of chemicals (including PFAS) impossible.
To ensure the continued supply of laboratory water we ask for a 12-year derogation for the sealing materials made from FKM and FFKM in Milli-Q® IQ 7000 series systems as well as in other laboratory water systems already in operation. The derogation should be reviewed after 7 to 8 years to assess the proceedings on the development of alternative materials or new technological solutions. Further, for the sustainable use of PTFE reactors in combination with UVC LEDs for the inactivation of bacteria instead of using mercury lamps, we also ask for a 12 year derogation including a review by the Commission after 7 to 8 years to enable us to utilize the technological progress on UVC LED efficiency and the development of technological feasible reactors concerning reflectivity, water movement (turbulence) in the reactor to ensure the same required quality of laboratory water that is needed.