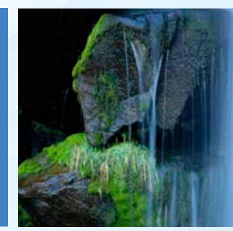
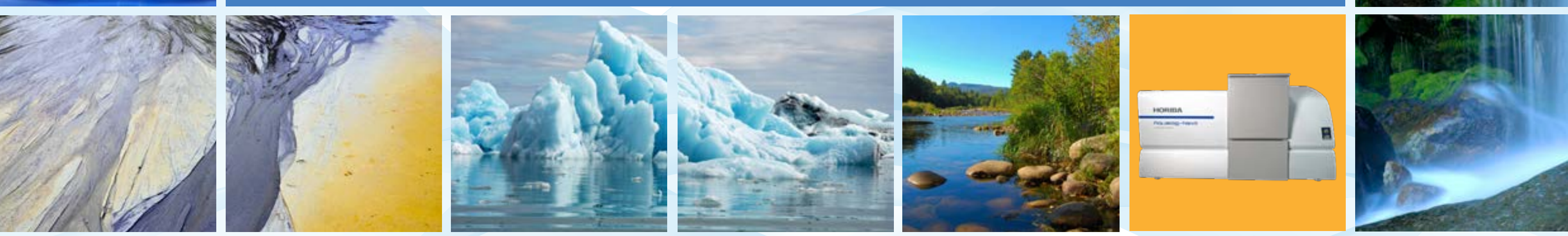
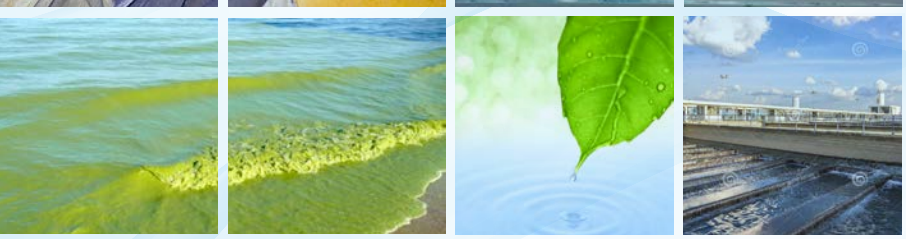
HORIBA

# Aqualog®–Next Environmental Water Research Analyzer







## The Gold Standard for Water CDOM Research

aqualog.com

# Aqualog®–Next

## 5th Generation of the World-Renowned Aqualog® for Water CDOM Research

### A faster and better spectrometer for colored dissolved organic matter (CDOM)

The Aqualog®-Next is the culmination of decades of HORIBA's industry-leading experience in the development of the highest level of spectrofluorometer performance in a convenient, affordable, easy-to-use benchtop model. Better than traditional slow scanning PMT fluorometers for EEMs, Aqualog®-Next simultaneously acquires absorbance and fluorescence EEMs with its patented A-TEEM™ design and ultra-fast CCD detector, acquiring complete A-TEEM fingerprints in seconds.

### Software

**EzSpec™** offers App icons to easily select and use dedicated data acquisition and analysis routines. The navigation of EzSpec includes Method Setup, Acquire, Process and Reporting to enable easy user interaction. EzSpec v2 now runs on a database, enabling easy filtering and searching of all files.

- Intuitive Navigation – Method Setup, Acquire, Process, and Reporting for seamless user interaction.
- Database Integration – Easily filter and search all files with EzSpec v2.
- Batch Processing – SampleQ for automated acquisition, processing, and ASCII file export.
- Advanced Data Tools – Inner-filter effect correction, Rayleigh masking, RSU normalization, and more.
- 3D-to-2D Profiling – Extracts X-Z axes for precise emission/excitation spectra analysis.
- Pass/Fail Application – Quick assessment of emission, excitation, absorbance, and %T spectra.
- Comprehensive Export Options – ASCII file export and PDF report generation for easy sharing.

**A-TEEM Direktor MVA Suite** offers step-by-step guided workflow for fluorescence A-TEEM data analysis.

- Predictive Modeling – Supports PARAFAC, PCA, and PLS models for classification and regression.
- User-friendly Interface – Drag-and-drop functionality and graphical tools for enhanced usability.

Eigenvector Inc. Solo for PARAFAC and other multivariate methods are also available, along with the exclusive HORIBA Multimodel Predictor (HMMP) toolbox itself, available as an add-in for Eigenvector Inc. Solo and PLS toolbox for applications in wine, food and water analysis.

### Two-in-one spectrometer captures more information simultaneously

Simultaneously acquiring absorbance and fluorescence EEMs, Aqualog®-Next captures information about fluorescent molecules, such as proteins, algae and BTEX, and it also acquires information about absorbing molecules and can provide parameters such as specific UV absorbance (SUVA).

### A-TEEM™ fingerprints provide better chemometric analysis

With absorbance-corrected fluorescence EEM fingerprints, the Aqualog®-Next provides A-TEEM fingerprints that are independent of fluorophore concentration over a wider dynamic range, thus offering more reliable quantitative component analysis than a traditional scanning fluorescence EEM.

### NIST-traceable validation

The Aqualog®-Next spectrometer is fully traceable to National Institutes of Standards and Technology (NIST) standard and certified reference materials (SRMs and CRMs) for both fluorescence and absorbance.

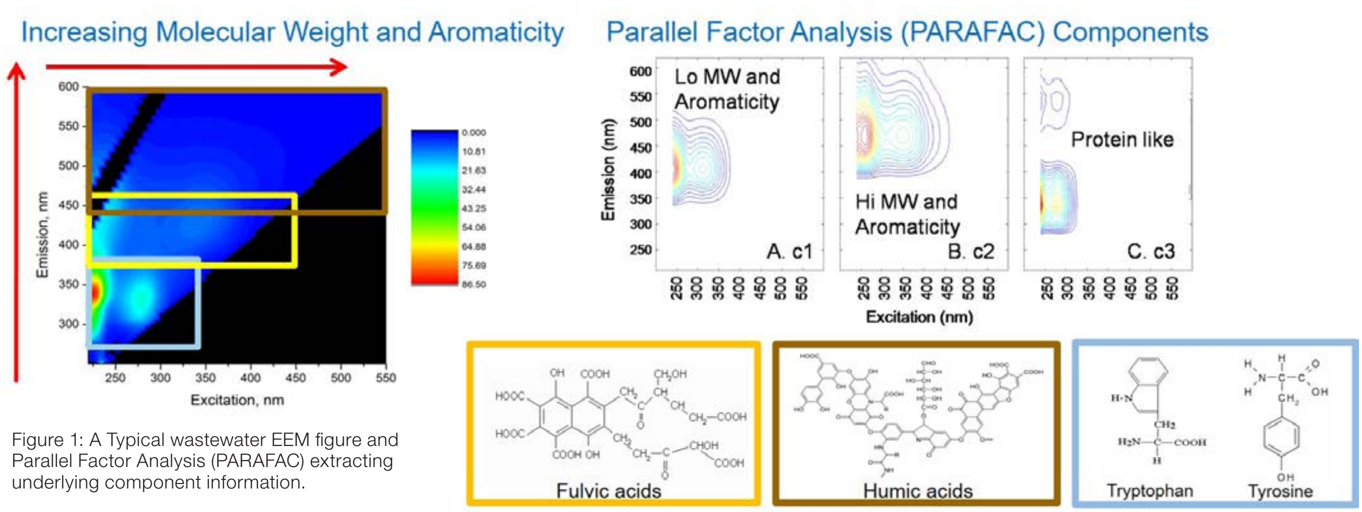



Figure 1: A Typical wastewater EEM figure and Parallel Factor Analysis (PARAFAC) extracting underlying component information.

# It's All About CDOM

Facing challenges like population growth and climate change, today's environmental water researchers are raising important questions on how to adapt technology and assess its effectiveness while continuing to protect public health.

Water researchers use the Aqualog®-Next A-TEEM spectrometer, a novel and valuable optical tool, to investigate fluorescent dissolved organic matter (DOM) characterization, with the aid of multivariate analysis, for example, parallel factor analysis (PARAFAC) that decomposes components and assigns scores (Figure 1). This provides key information on DOM composition, allowing researchers to track the seasonal and operational trends of specific fractions of DOM in the source water and throughout the drinking water treatment plant. Raw water sampling allows utilities to understand how surface water quality is related to seasonal changes. Sampling throughout the plant allows utilities to understand how operations impact removal of specific fractions of DOM.

Of these fractions, humic and fulvic acids comprise the majority in most surface water sources. Humic and fulvic acids both contain molecules in the 200 - 600 DA range revealed by FT-ICR-MS analysis. The primary differences are that humic acids have a greater C content and a higher aromatic content. Fulvic acids have a higher O content in the form of carboxyl group (COOH) and phenolic hydroxyl groups (Ar-OH). The abundance of the latter groups in fulvic acid molecules is what makes them soluble via hydrogen bonding with water molecules. Humic acids, which have a lower content of COOH and Ar-OH groups are more susceptible to coagulants, in particular if $Al^{+3}$ or $Fe^{+3}$ are used, because they become cross linked into large pseudo molecules and become very hydrophobic.

The effectiveness of all water and wastewater treatment processes is impacted by organic matter, so no single treatment method can remove all the types of organic carbon present in these waters, and methods of improved characterization of organic matter are therefore needed at various stages of water and wastewater treatment. While surrogate measures of UVA254, total and dissolved organic carbon (TOC/DOC), and chemical oxygen demand (COD) indicate trends, they inadequately portray the character and composition of the organic matter removed and/or transformed at each treatment stage or reuse process.

Protein-like compounds are another significant component of natural organic matter present in most surface water sources. They are also known to be associated with the presence of municipal wastewater and microbially available substrates. Compared to humic and fulvic acids, the protein-like compounds have a lower affinity to coagulants. Since many DOM components are disinfection byproducts (DBP) precursors, halogenated disinfectants, such as chlorine, can react with the DBP precursors to form unwanted DBPs, which include toxic substances, such as trihalomethanes (THMs) and haloacetic acids (HAAs). Because these substances are potentially carcinogenic and are regulated by the US EPA, their formation should be controlled by properly managing and optimizing the water treatment process.

# The Gold Standard for Water Research

## A sampling of our customers around the world

### Environmental Researchers

US Environmental Protection Agency (US EPA)
US Geological Survey (USGS) Water Science Center
US Naval Research Laboratory
National Institute of Standards and Technology (NIST)
National Aeronautics and Space Administration (NASA)
National Oceanic and Atmospheric Administration (NOAA)
Woods Hole Oceanographic Institution
Stroud Water Research Center
Trussell Technologies
Vietnam Environment Administration
National Laboratory for Civil Engineering (Portugal)
Korea Institute of Civil Engineering and Building Technology (South Korea)
Arizona State University
Chinese Academy of Sciences (China)
Colorado School of Mines
Columbia University
Florida International University
Florida State University
Georgia Institute of Technology
Harbin Institute of Technology (China)
Indiana University
Kangwon National University (South Korea)
King Abdullah University of Science and Technology (Saudi Arabia)
Kobe University (Japan)
Louisiana State University
Michigan Technological University
New Mexico State University
Northeastern University
Oregon State University
Rutgers University
San Diego State University
Seattle University
Sejong University (South Korea)
Sichuan University (China)
Southwest University (China)
Swedish University of Agricultural Sciences (Sweden)
The Ohio State University
The University of Vermont
Tongji University (China)
Umeå University (Sweden)
University of Alaska
University of Alberta (Canada)
University of East Anglia (UK)
University of Extremadura (Spain)
University of Maryland, Center for Environmental Science
University of Massachusetts at Amherst
University of Michigan
University of Minnesota
University of Montana
University of New Orleans
University of Science of Technology of China (China)
University of South Africa (South Africa)
University of Western Ontario (Canada)

### Water Companies

American Water
Chelsea Technologies Group
Doosan Heavy Industries and Construction
Eskom (South Africa)
Hazen and Sawyer
Kurita Water (Japan)
Public Utilities Board (PUB) of Singapore
Sabesp (Brazil)
Suez (Worldwide)
WET Labs

### Municipal Water Facilities

City of Akron
City of Philadelphia Water Department
City of Sandusky
EMASESA Water Treatment
Sydney Australia Water Laboratory
Metrowater Recovery
City of Wheeling Water Department
Denver Water
Hampton Roads Sanitation District
Las Vegas Valley Water District
Louisville Water Company
Metropolitan Water District of Southern California
Middlesex Water Company
Orange County Water District
Umgeni Water - Amanzi (South Africa)
West Basin Municipal Water District Water Recycling Facility

# Aqualog®-Next Applications

### Drinking Water for EPA Compliance

Environmental water researchers use HORIBA's patented technology method in the Aqualog®-Next to track fluorescence fingerprints of NOM in water, also known as the precursors of the DBPs. This allows them to quickly predict, identify and optimize the organics removal, in order to mitigate the DBPs formation, and to ensure compliance with increasingly stringent drinking water quality regulations.

Photo credit:Tom Archer

### Harmful Algal Blooms (HABs)

HABs are a global concern limiting access to numerous bodies of water for recreational use (fishing, boating, swimming etc.,) and water utilities. They are also associated with extreme malodorous conditions and unsightliness. Environmental water researchers use the HORIBA Aqualog®-Next to monitor fluorescence signatures of planktonic algal cells, as well as organic matter derived from HABs which can be an indicator of upcoming blooms and DBP formation.

### Membrane Fouling in Advanced Water Treatment

Potable reuse, wastewater recycling processes can both positively impact water availability and water contamination. The technologies often involved are membrane treatments, however, membrane fouling occurs when contaminants deposit on the surface of a membrane, which leads to deterioration of membrane performance and decrease in treatment efficiency. In these studies, researchers use the Aqualog®-Next to investigate specifically how the performance and fouling of membrane treatments, is affected by the design and operation of the upstream wastewater effluent. Monitoring the removal of organic micropollutants by membrane treatments, such as reverse osmosis, or by ozone, coupled with biological filtration, are also both important applications.

### Climate Change and NOM in Aquatic Environments

Aqualog®-Next is being used in a wide range of different aquatic environments, from cold arctic regions to boreal lakes and streams, and from ice glaciers to coastal water, to help environmental researchers understand the biogeochemical origin of climate change. By tracking the emerging patterns of global CDOM distribution, researchers can then determine the contribution of carbon from different origins into the CDOM pool.

### Petroleum and Oil Products Spills

Global drinking water sources remain prone to carcinogenic petroleum product contaminations due to lack of detection capacity at, or before treatment plant intake. The Aqualog®-Next A-TEEM method provides a reliable optical detection of these compounds at low quantities, while discriminating from the highly absorbing and fluorescent backgrounds of natural Dissolved Organic Matter (DOM) components. Environmental water researchers use the HORIBA Aqualog®-Next to monitor fluorescence signatures of benzene, toluene, ethylbenzene and xylene (BTEX), as well as polycyclic aromatic hydrocarbons (PAHs), which represent typical water soluble fractions of petroleum products, as an early warning detection of petroleum and oil product spills.

ASTM INTERNATIONAL

Standard D8431
Developed with Aqualog and A-TEEM

Standard Test Method for Detection of Water-soluble Petroleum Oils by A-TEEM Optical Spectroscopy and Multivariate Analysis

# Unique Aqualog®-Next A-TEEM™ Benefits

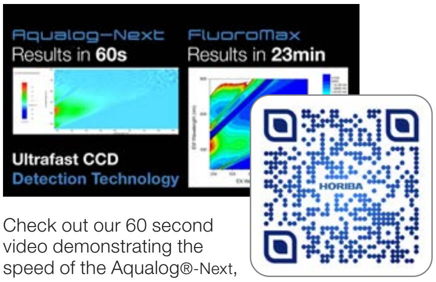
## Not just a scanning fluorometer for EEMs, but a much faster and better A-TEEM™ spectrometer for colored dissolved organic matter (CDOM)

### A-TEEM versus a Traditional Scanning EEM Fluorometer

Aqualog®-Next represents the future of analytical benchtop fluorescence spectroscopy by providing faster, better and more accurate information than traditional scanning fluorometers.

Traditional scanning spectrofluorometers have been widely used to collect a molecular fingerprint, in the form of a fluorescence excitation emission matrix, or EEM. With a scanning spectrofluorometer, this data set is acquired by sequentially scanning a series of emission spectra, at varying excitation wavelengths, and then reconstructing the resultant 3D data set. This three-dimensional data set can be used with third party multivariate analysis software for component analysis, as is done with other analytical techniques such as FTIR, HPLC and MS. There are, in fact, many scientific papers published citing the use of scanning spectrofluorometers for fluorescence EEM component analysis in the water research field. But, if an EEM provides more information for a scientist, why aren't EEM publications growing faster? Primarily because a PMT scanning fluorometer is very slow to acquire an EEM, but also because conventional EEM measurements can be distorted by absorbance artifacts known as inner filter effects.

| | Aqualog®-NEXT A-TEEM | Scanning EEM |
|---|---|---|
| Acquisition Speed | Fast, 1 minute | Slow, 45 minutes |
| Spectroscopic Method | Fluorescence & Absorbance | Fluorescence only |
| Emission Detector | CCD camera | Photon multiplier tube (PMT) |
| Inner Filter Effects Correction | Automatic, real-time | Need a second instrument |
| Multi-block for Enhanced Multivariate Analysis | Yes | No |




Check out our 60 second video demonstrating the speed of the Aqualog®-Next, compared to a scanning PMT fluorometer.

With ultrafast CCD detection technology, HORIBA Aqualog®-Next solves the serious speed limitations of scanning spectrofluorometers so that an entire fluorescence EEM can be acquired in mere seconds to minutes faster than traditional PMT-based fluorometers, depending on the sample.

Below is a good example to show how even a small concentration difference in a single molecule, gallic acid, can have a significant effect on the shape of an EEM fingerprint, but with proper IFE correction, an A-TEEM fingerprint remains the same. With our new A-TEEM technology you can easily and effectively identify, quantify and understand individual organic compounds in complex mixtures in minutes.

HORIBA has solved both the scan speed limitations and inner-filter effect distortions so that the A-TEEM technique also collects absorbance of the same sample at the same time as the fluorescence, and uses the absorbance to correct EEMs for the inner filter effect (IFE).

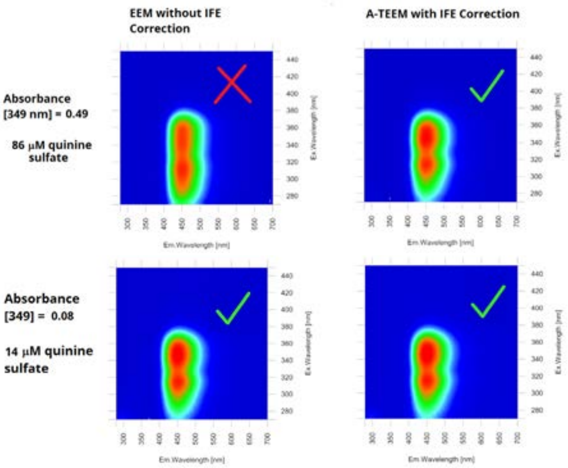
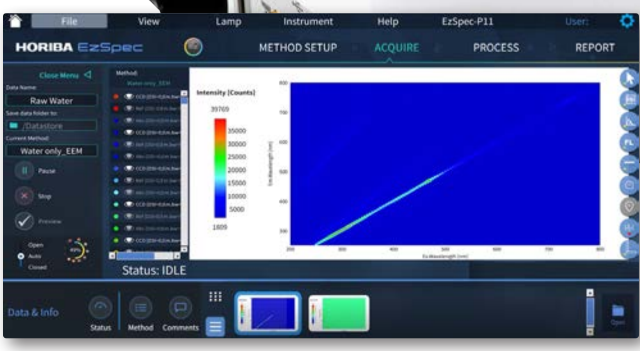
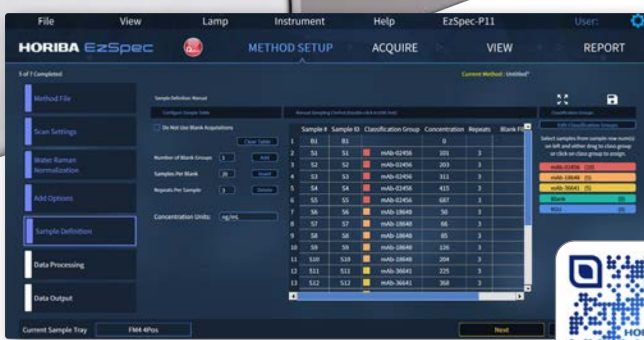



Figure 2: Fluorescence Excitation Emission Matrices of two concentrations of quinine sulfate in tonic water diluted in 0.1 M perchloric acid (aq.) with and without inner-filter effect corrections applied.


Check out our 2-minute video showcasing EzSpec™ in action

## Accessories

### Fast-03 Autosampler Accessory

The Fast-03 can be configured to use a variety of sample vials and racks to meet your application needs, and enables complete temperature control. Sample vial repeats and injection volumes are easily facilitated with the Aqualog®-Next EzSpec™ software, which also offers preconfigured blank files.

All data files can be exported with ISO-formatted time-date stamping and user-configurable Sample ID and repeat codes. All aspects of the Fast-03 hardware control are at your fingertips, with key real-time access features to facilitate the configuration and execution of your batch experiments, as well as priming, cleaning and maintenance.

### Additional Accessories:

- 4-position thermostatted cuvette holders
- 4-position Peltier thermostatted cuvette holders
- External water bath for temperature control
- Remote fiber optics for external samples
- Solid sample holders

## Aqualog®-Next Specifications

| Fluorescence Hardware | |
|---|---|
| Light source | Extended-UV:<br>150W vertically mounted xenon arc lamp |
| Excitation range | 0-800 nm, 200-800 intensity corrected |
| Excitation bandpass | 5 nm |
| Excitation monochromator | Subtractive double monochromator |
| Excitation gratings | 1200 gr/mm, 250 nm blaze |
| Excitation wavelength accuracy | ±1 nm |
| Emission range | 250-800 nm |
| Emission grating | 285 gr/mm; 350 nm blaze |
| Hardware pixel binning | 4.64, 2.32, 1.16, 0.58 nm/pixel |
| Emission bandpass | 5 nm |
| Emission spectrograph | Fixed, aberration-corrected<br>140 mm focal length |
| Emission detector | TE-cooled back-illuminated CCD |
| Emission integration time | 5 ms - 60 s |
| CCD gain options | 2.25 e-/cts in high gain, 4.5 e-/cts in medium gain,<br>9 e-/cts in low gain |
| Sensitivity | Water-Raman SNR > 20,000:1 (RMS method)<br>(350 nm excitation, 30s integration) |
| Sample Holder | Rapid Peltier Controlled Single Position Sample Holder |
| Weight | 32.72 kg (72 lbs) |
| Dimensions | LWH (618 x 435 x 336 mm); (24" x 17" x 13") |

| Absorbance Hardware | |
|---|---|
| Scanning range | 200-800 nm |
| Bandpass | 5 nm |
| Slew speed | Maximum 500 nm/s |
| Optical system | Corrected single-beam |
| Detector | Si photodiode |
| Wavelength accuracy | ±1 nm |
| Wavelength repeatability | +/- 0.5 |
| Photometric accuracy | +/- 0.01 AU from 0 to 2 AU |
| Photometric stability | <0.002 AU per hour |
| Photometric repeatability | +/- 0.002 AU (0 to 1 AU)l |
| Stray light | Measured with KI, NaNO3, and Acetone |
| Performance validation tests | NIST Fluorescence Standard Reference Materials for spectral calibration and correction (SRMs: 2940, 2942, 2943)<br>Starna® Standard Reference Material for Quinine Sulfate<br>Fluorescence Emission Spectral Correction (RM-QS00)<br>Water Raman Signal-to-Noise evaluation (RM-H20)<br>Spectrophotometry (RM-020610HLACKISN/CW/15-R)<br>US Pharmacopoeia (USP) 857 compliant absorbance photometric accuracy/linearity tests with (Starna) NIST SRM 935a potassium dichromate; stray light tests with potassium iodide (KI), sodium nitrite (NaNO2), acetone |

*“The University of South Africa’s Nanotechnology and Water Sustainability (NanoWS) research unit has been at the forefront of water research in South Africa, developing and optimizing various materials for removal of various pollutants from our different water sources. We continue to use the Aqualog® and Eigenvector for the complete quantitative spectral profile of all colored and fluorescent dissolved organic carbon (DOC) components. The service team at HORIBA also provides professional and comprehensive after sales care of their customers, availing their expertise and support throughout our research, thus impacting the quality of life of our people positively.”*

Dr. Thabo T.I. Nkambule
Nanotechnology & Water Sustainability
(NanoWS) Research Unit
College of Science
University of South Africa

*“In my research, I use EEM/PARAFAC data generated by the HORIBA Aqualog® instrumentation/software to understand better water quality and organic carbon distribution throughout the drinking water and wastewater treatment industries. My background is in government, academia, and industrial labs. I encourage academic environmental science and engineering programs to obtain this instrumentation to prepare students for jobs in the water industry. In addition, the Aqualog instrument (dual UV-Vis and fluorescence) obtains data much more rapidly using a single instrument than traditional spectrofluorometric instrumentation, such that experiments are achieved within limited academic student-lab timeframes.”*

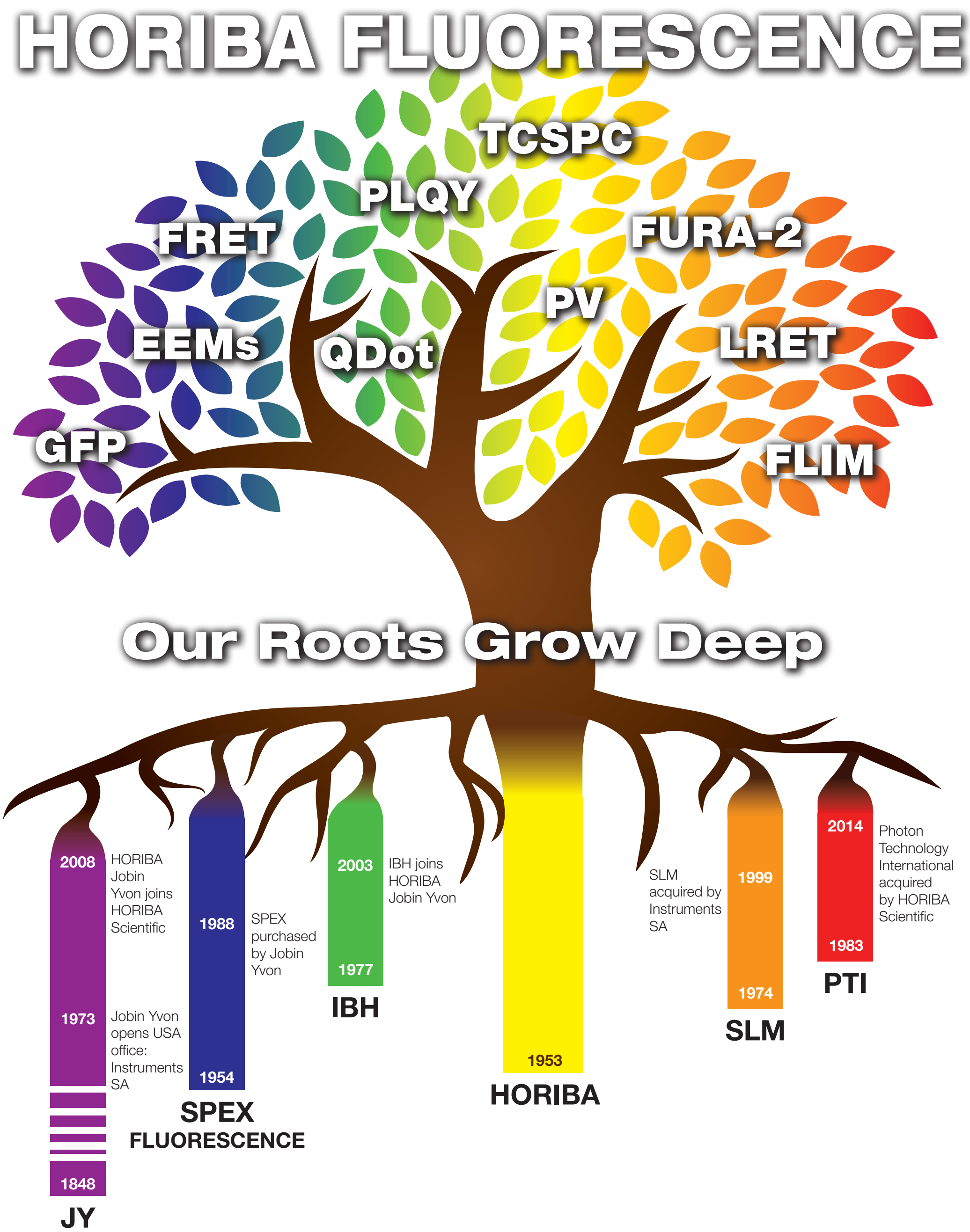
Martha J.M. Wells, Ph.D.
Owner/Consulting Chemist, EnviroChem Services,
Emeritus Professor of Chemistry
Tennessee Technological University

A-TEEM™
MOLECULAR FINGERPRINTING

## Beyond Water Research

Aqualog®-Next was designed for quantitative and predictive water analysis, and it is ideal for the task. However, A-TEEM molecular fingerprinting has proven to be an invaluable tool in a wide variety of industrial applications, such as Biopharma QC/QA and process, wine and spirits, olive oils and much more. For more information about other applications of A-TEEM spectroscopy visit www.a-teem.com.

*Some Aqualog A-TEEM chemometrics analysis presented here are derived from Eigenvector Research Incorporated, Solo software.*




**Acronyms**

| | | | |
|---|---|---|---|
| A-TEEM | Absorbance -Transmission and Fluorescence Excitation and Emission Matrix | HABs | Harmful Algal Blooms MCL Maximum Contaminant Level |
| BTEX | Benzene, Toluene, Ethylbenzene and Xylenes | MW | Molecular Weight |
| DBPs | Disinfection By-product(s) | NOM | Natural Organic Matter |
| DOC | Dissolved Organic Carbon | PAHs | Polycyclic Aromatic Hydrocarbon |
| EEM | Excitation and Emission Matrix | PARAFAC | Parallel Factor Analysis |
| EPA | Environmental Protection Agency | SUVA | Specific Ultraviolet Absorbance |
| HAA | Haloacetic Acids | THM | Trihalomethanes |
| | | TOC | Total Organic Carbon |

**HORIBA**

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Printed July 2025