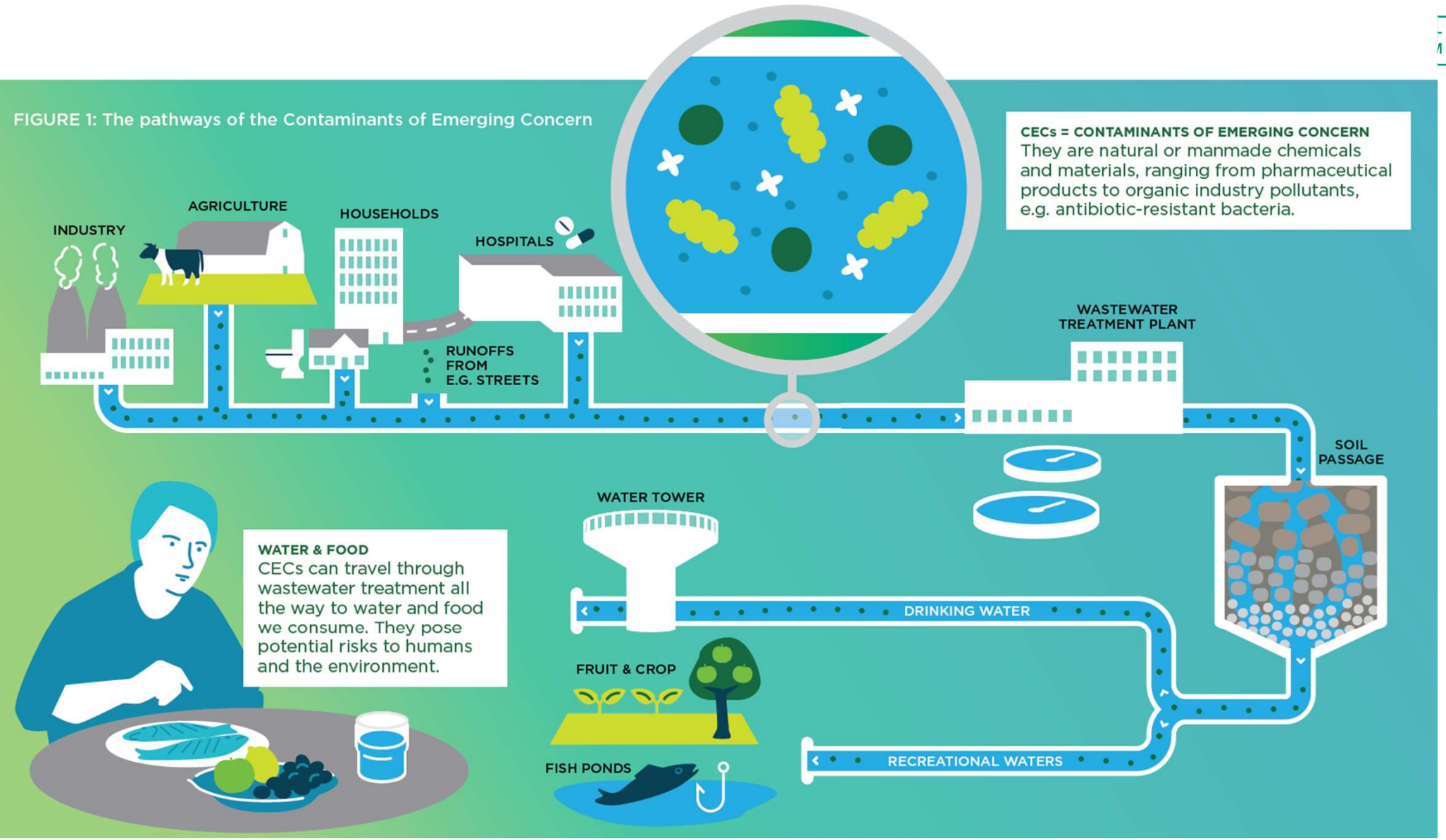
Online surveillance and control of emerging contaminants

Agnieszka Cuprys



Water JPI, Policy Brief, 22 October 2018

Water quality guidelines

Watch list of substances for Union-wide monitoring as set out in Article 8b of Directive 2008/105/EC

Name of substance/group of substances	CAS number (1)	EU number (2)	Indicative analytical method (3) (4)	Maximum acceptable method detection limit (ng/l)
Metaflumizone	139968-49-3	604-167-6	LLE-LC-MS-MS or SPE–LC-MS-MS	65
Amoxicillin	26787-78-0	248-003-8	SPE-LC-MS-MS	78
Ciprofloxacin	85721-33-1	617-751-0	SPE-LC-MS-MS	89
Sulfamethoxazole (5)	723-46-6	211-963-3	SPE-LC-MS-MS	100
Trimethoprim (5)	738-70-5	212-006-2	SPE-LC-MS-MS	100
Venlafaxine and O-desmethylvenlafaxine (6)	93413-69-5 93413-62-8	618-944-2 700-516-2	SPE-LC-MS-MS	6
Azole compounds (7)			SPE-LC-MS-MS	
Clotrimazole	23593-75-1	245-764-8		20
Fluconazole	86386-73-4	627-806-0		250
Imazalil	35554-44-0	252-615-0		800
Ipconazole	125225-28-7	603-038-1		44
Metconazole	125116-23-6	603-031-3		29
Miconazole	22916-47-8	245-324-5		200
Penconazole	66246-88-6	266-275-6		1 700
Prochloraz	67747-09-5	266-994-5		161
Tebuconazole	107534-96-3	403-640-2		240
Tetraconazole	112281-77-3	407-760-6		1 900
Dimoxystrobin	149961-52-4	604-712-8	SPE-LC-MS-MS	32
Famoxadone	131807-57-3	603-520-1	SPE-LC-MS-MS	8,5

UNIVERSITAS

Tab. 10: List of substances proposed for the first Voluntary Groundwater Watch List

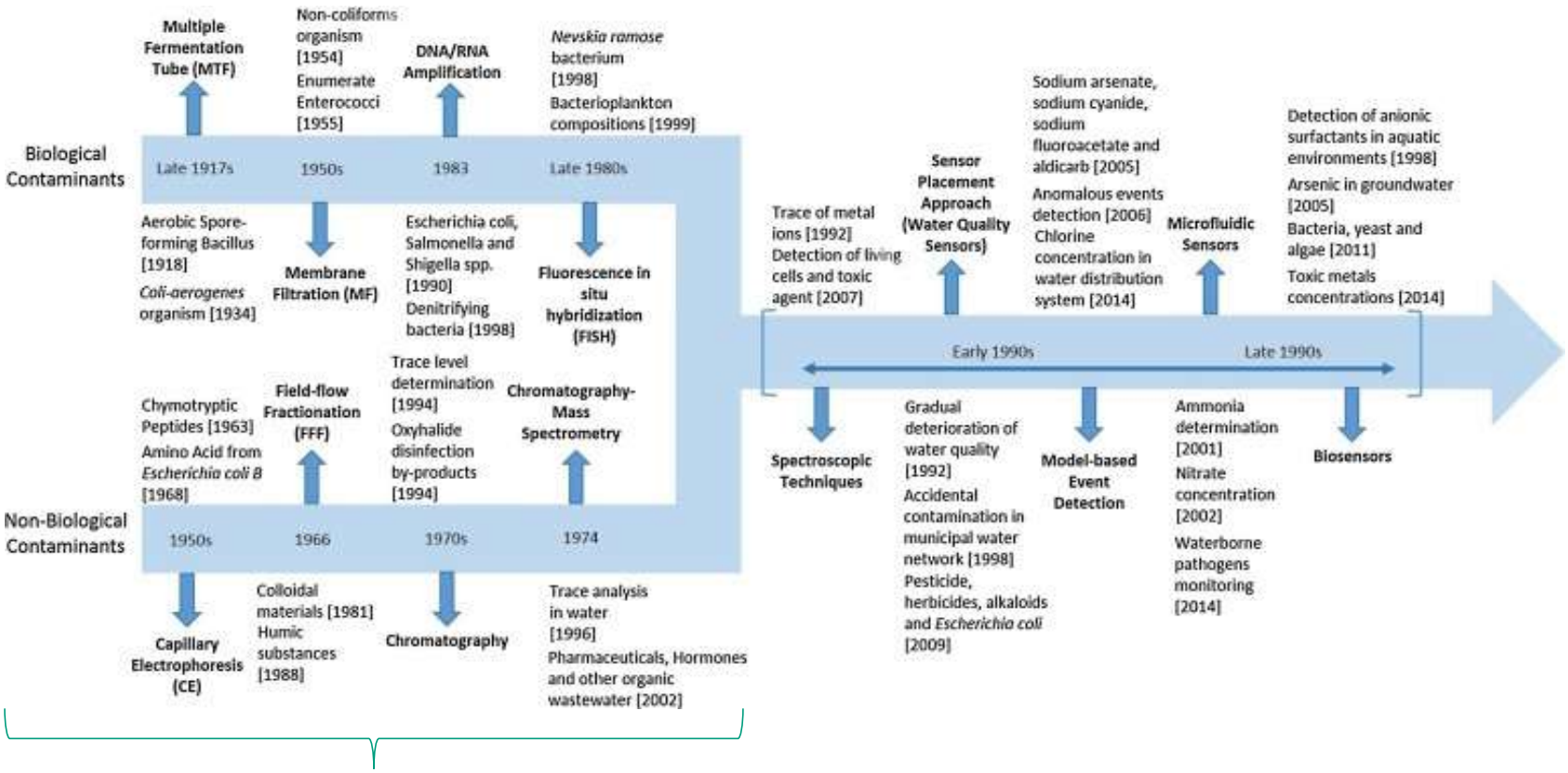
Substance Name	Group of substance	Acronym	Sub-group
Perfluorododecanoic Acid (L)	**PFAS**	**PFDoA**	**PFCAs**
Perfluoroundecanoic Acid (L)	**PFAS**	**PFUnA**	**PFCAs**
Clopidol	Pharmaceutical		
Crotamiton	Pharmaceutical		
Amidozoic Acid	Pharmaceutical		
Sulfadiazin	Pharmaceutical		
Primidone	Pharmaceutical		
Sotalol	Pharmaceutical		
Ibuprofen	Pharmaceutical		
Erythromycin	Pharmaceutical		
Clarithromycin	Pharmaceutical		
Further candidates			
4:2 Fluortelomerphosphatemonoester (S)	PFAS	**4:2 monoPAP**	**monoPAP**
Perfluorodecyl Phosphonic Acid (L)	PFAS	**PFDPA**	**PFPAs**
Perfluorooctyl Phosphonic Acid (L)	PFAS	**PFOPA**	**PFPAs**
6:2 Fluortelomerphosphatemonoester (S)	PFAS	**6:2 monoPap**	**monoPAP**

Drinking Water Directive

Chemical parameters

Parameter	Parametric value	Unit
⇨ Beta-estradiol (50-28-2) ⇦	⇨ 0,001 ⇦	⇨ µg/l ⇦
⇨ Bisphenol A ⇦	⇨ 0,01 ⇦	⇨ µg/l ⇦
⇨ PFAS ⇦	⇨ 0,10 ⇦	⇨ µg/l ⇦
⇨ PFASs - Total ⇦	⇨ 0,50 ⇦	⇨ µg/l ⇦

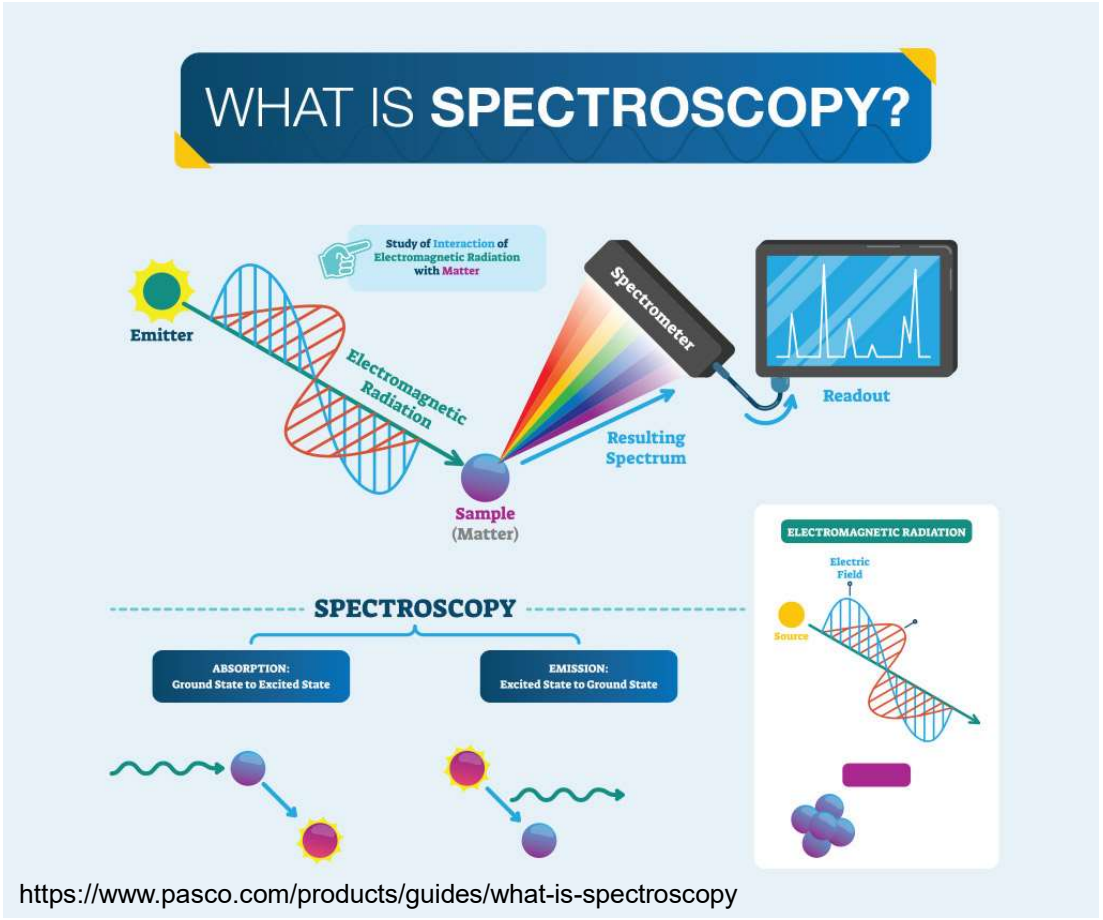
Evolution of contaminant detection techniques in water analysis application



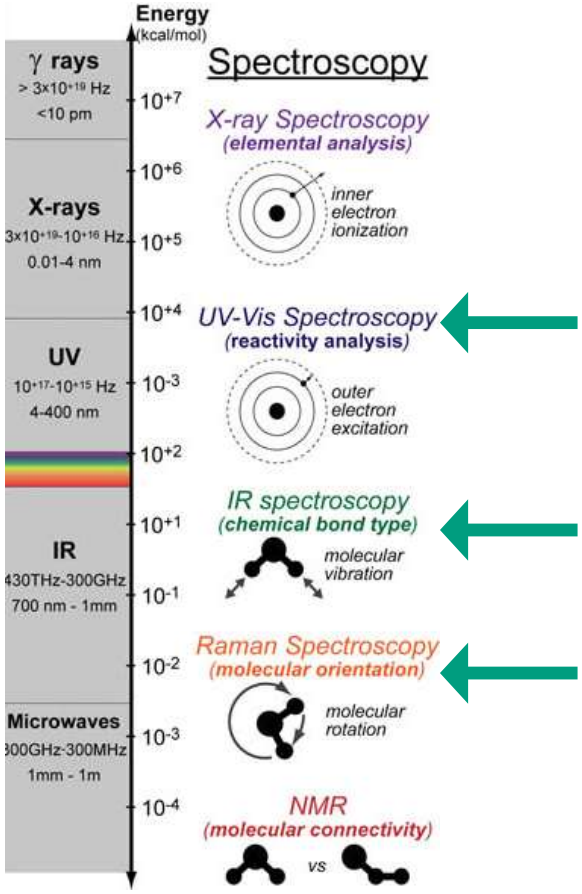
Laboratory-based methods

Zulkifli et al. (2018), https://doi.org/10.1016/j.snb.2017.09.078

Spectroscopic techniques

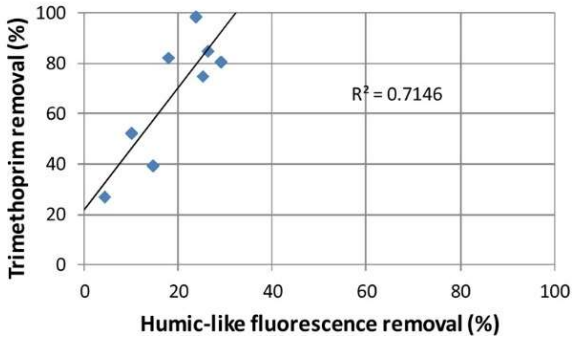


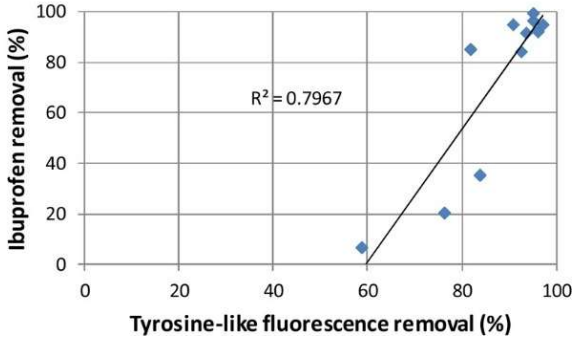
https://www.pasco.com/products/guides/what-is-spectroscopy



Spectroscopic techniques

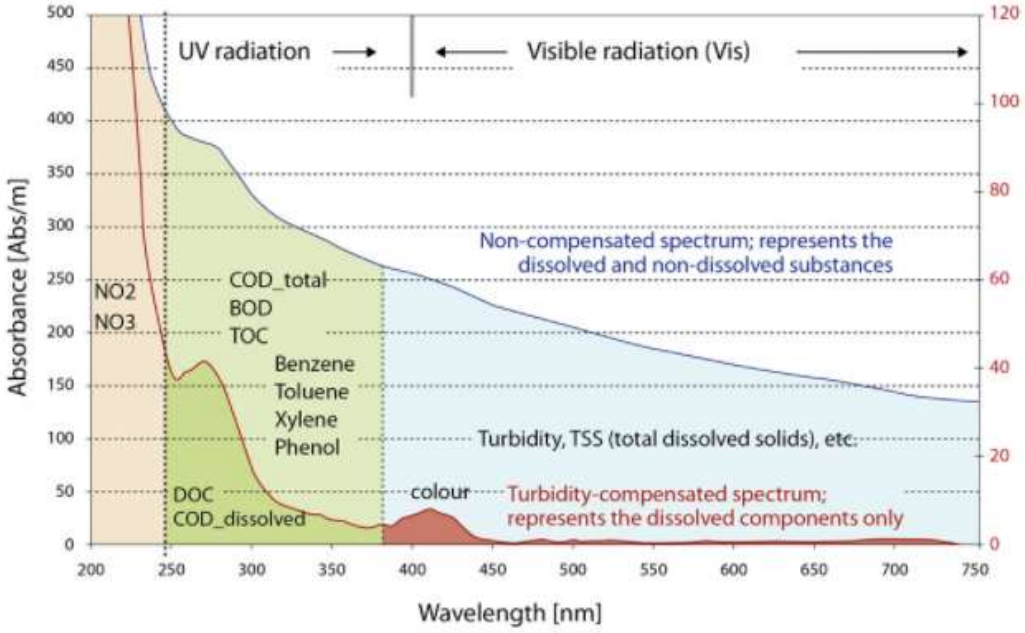
Monitoring the removal of emerging trace organic contaminants in wastewater treatment plants using fluorescence EEMs

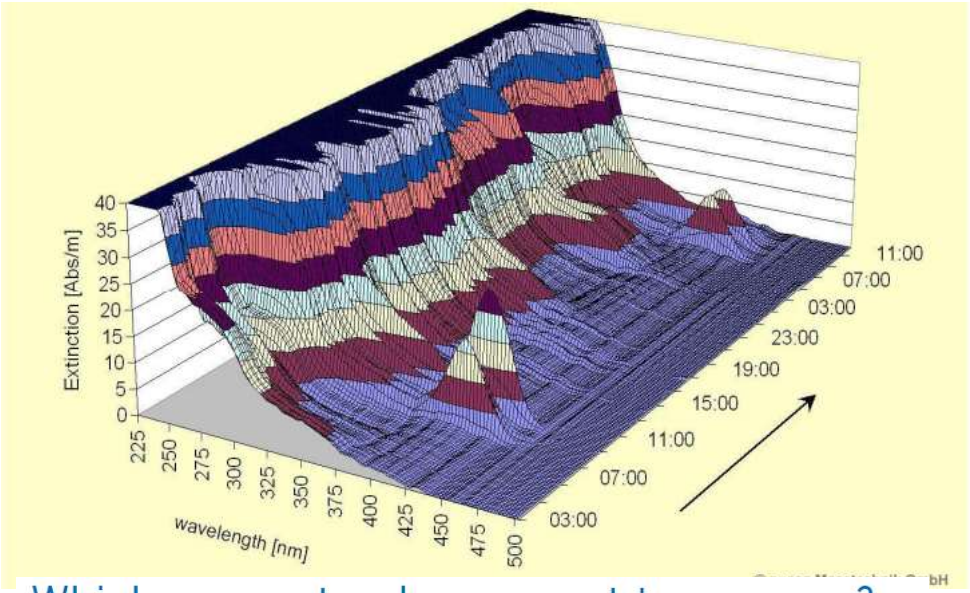




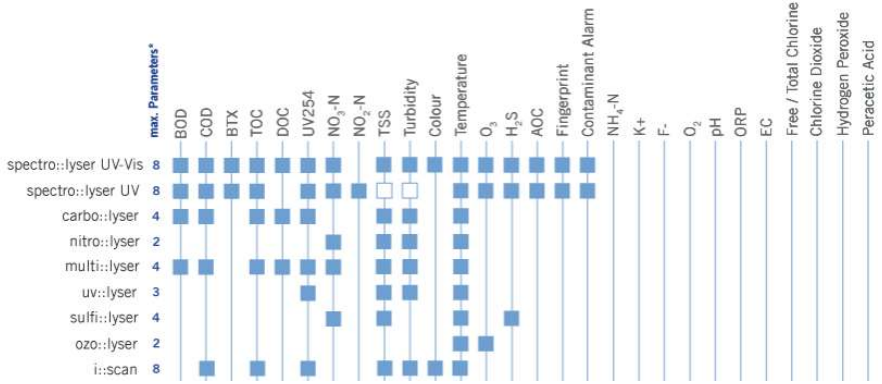
Sgroi et al. (2017), https://doi.org/10.1016/j.jhazmat.2016.05.035

Spectroscopic techniques





Which parameter do you want to measure?



Spectroscopic techniques

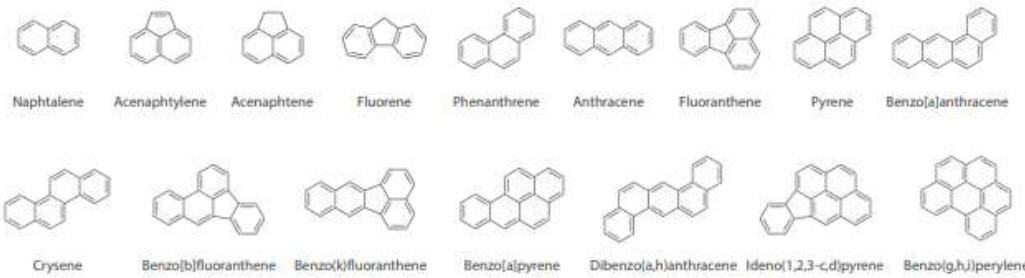
Fluorometer for measurements of PAH (polycyclic aromatic hydrocarbons)

Benefits

- Without sampling and preparation of test samples
- Real time sensor
- Without reagents
- High sensitivity and selectivity
- Optical window with nano coating

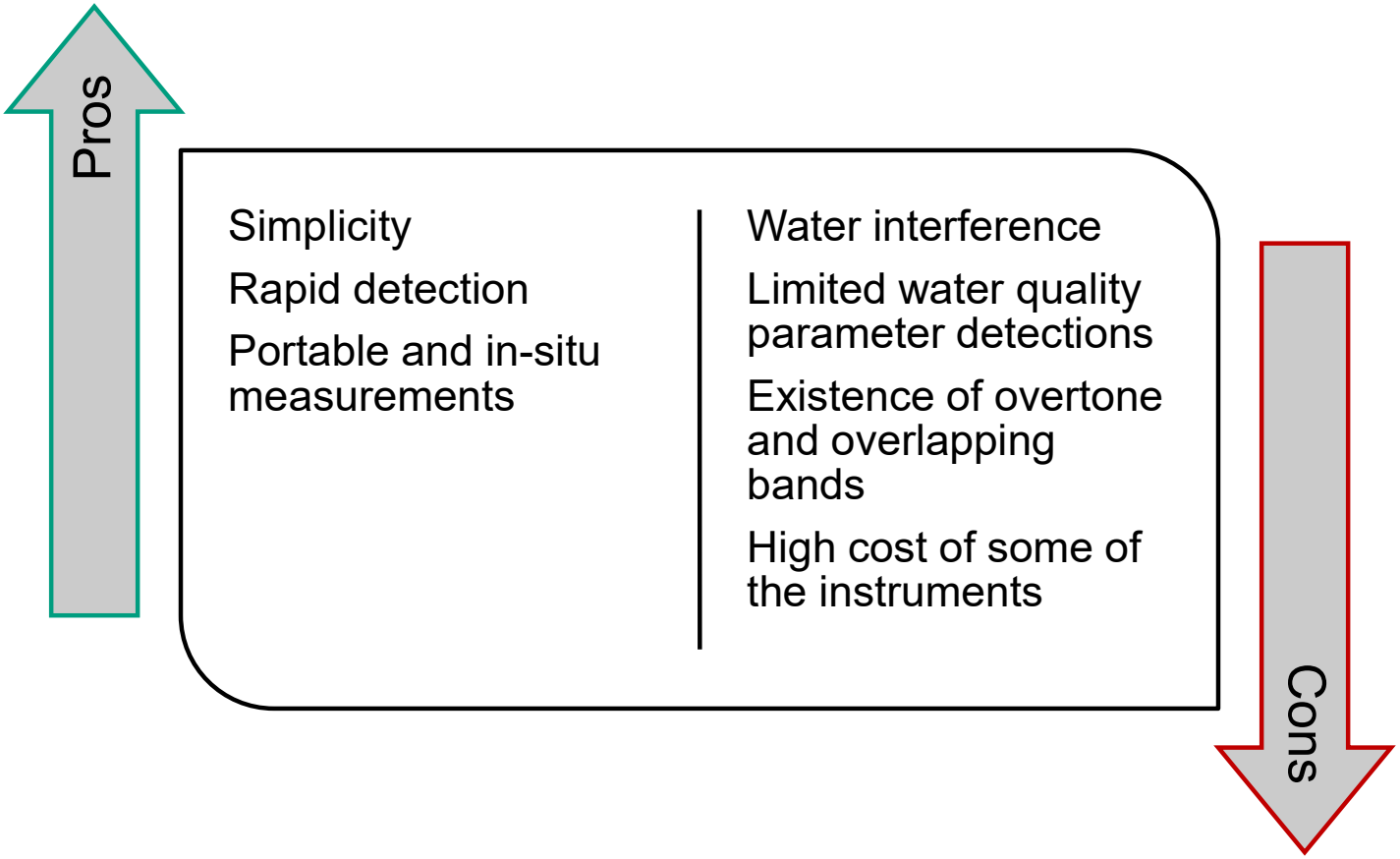
Applications

- Drinking water
- Wastewater
- Airports
- Cooling water
- Desalination plants
- Refineries
- Pipeline monitoring
- Bilge water monitoring
- Exhaust gas cleaning with approval for ship use according to IMO regulation MEPC.184(59)



https://www.trios.de/en/enviroflu.html

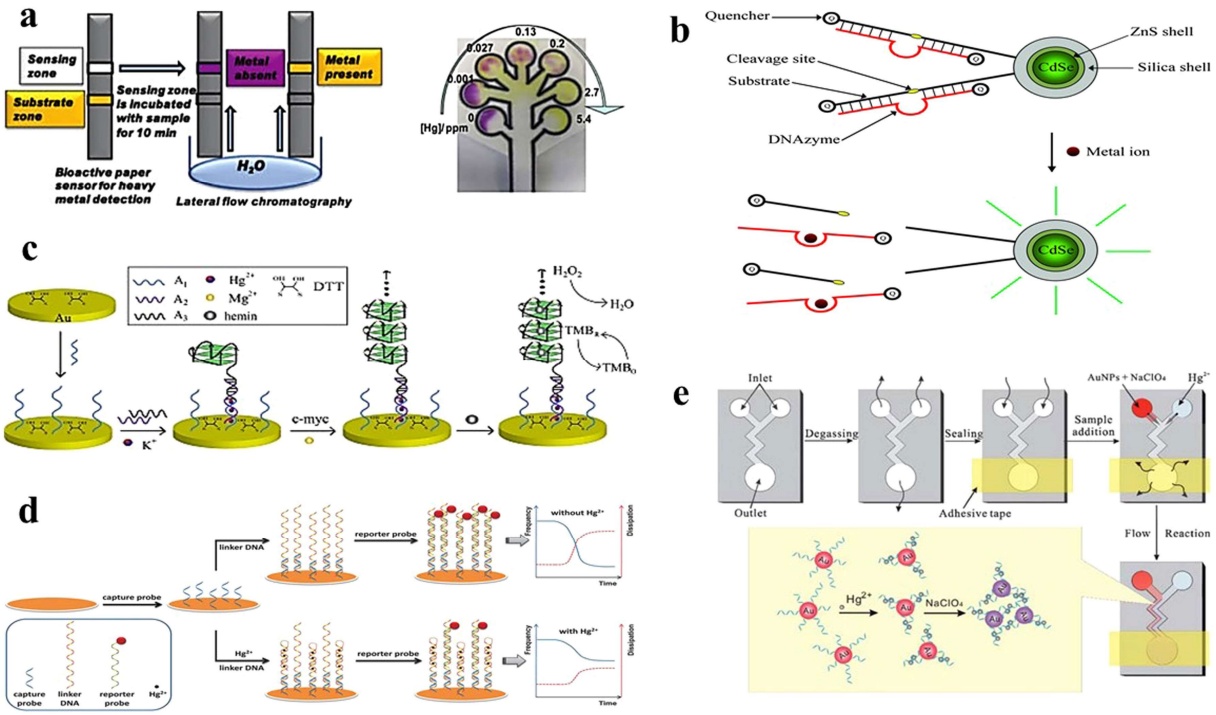
Spectroscopic techniques



Biosensors

CONTAMINANT → MOLECULAR SIGNAL → TRANSDUCER →

MOLECULAR SIGNAL
Enzyme, whole cell, antibody, nucleic acid

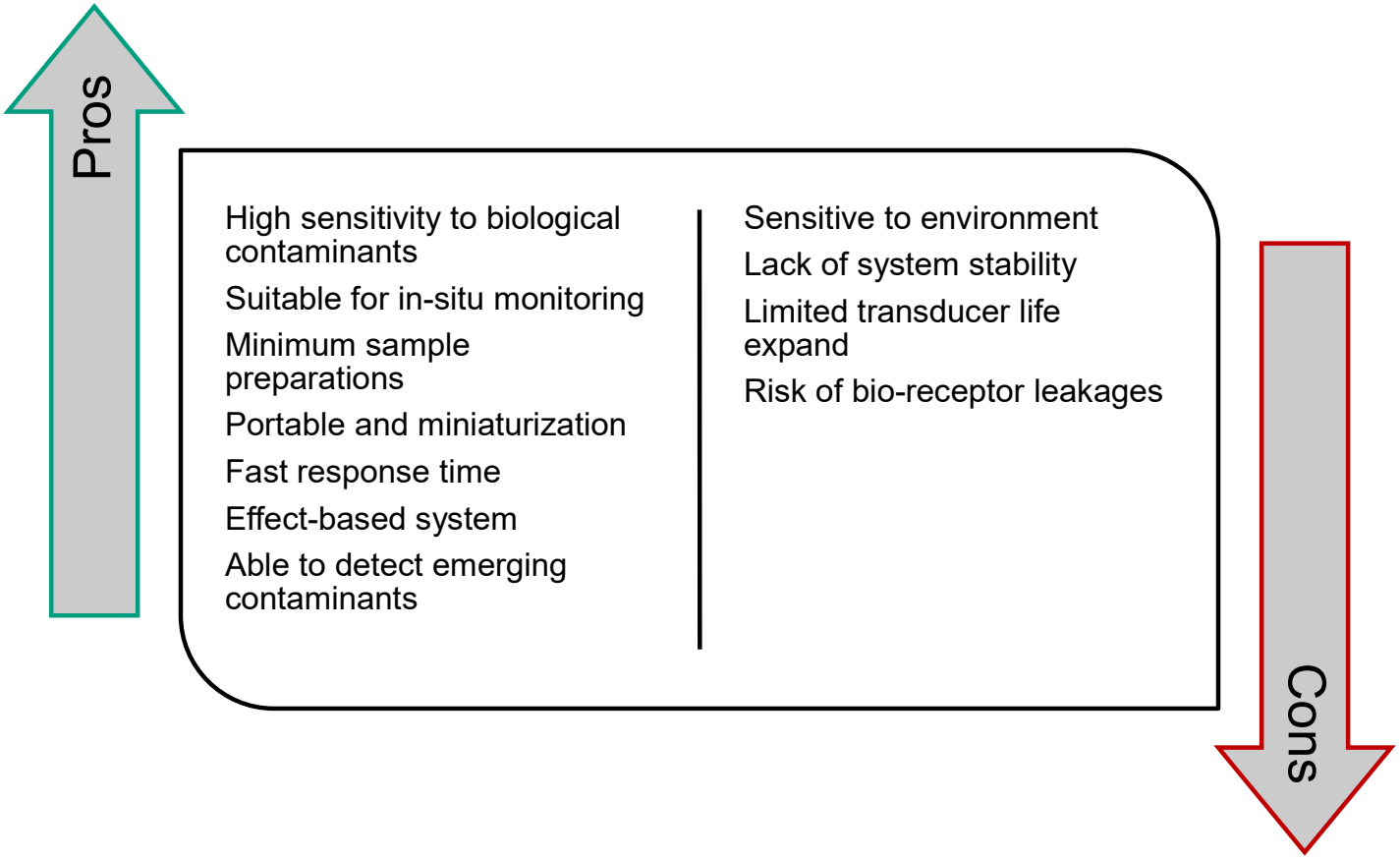


Biosensors for detection of heavy metals

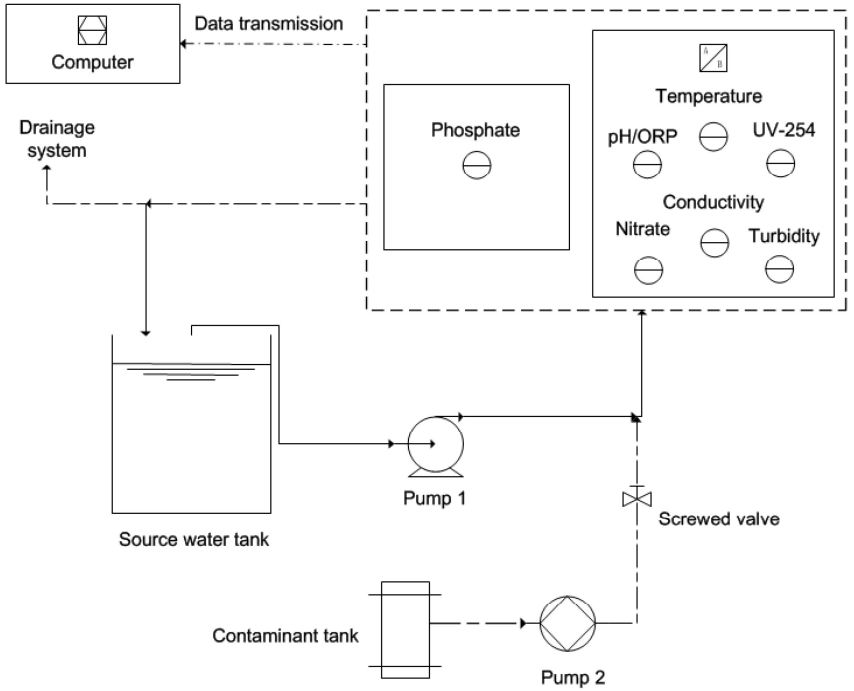
(a) Schematic description for detection principle of β-GAL based optical biosensor for sensing of Hg ion with various concentrations (Hossain and Brennan, 2011),
(b) Schematic diagram quantum dots-DNAzyme based fluorescence resonance energy transfer nanobiosensor for detection of metal ion (Wu et al., 2010),
(c) Schematic plane of the working mechanism of a label-free guanine nanowire amplification-based Hg^{2+} biosensor (Huang et al., 2016),
(d) Schematic presentation of AuNPs-enhanced quartz crystal microbalance with dissipation monitoring sensor for Hg^{2+}, composed of a DNA capture probe, a linker DNA, and a DNA reporter sequence tagged with GNPs (Chen et al., 2011a), and
(e) The schematic presentation of a power-free biosensing system for colorimetrically detection of Hg^{2+} by using modified Au nanoparticles (He et al., 2008).

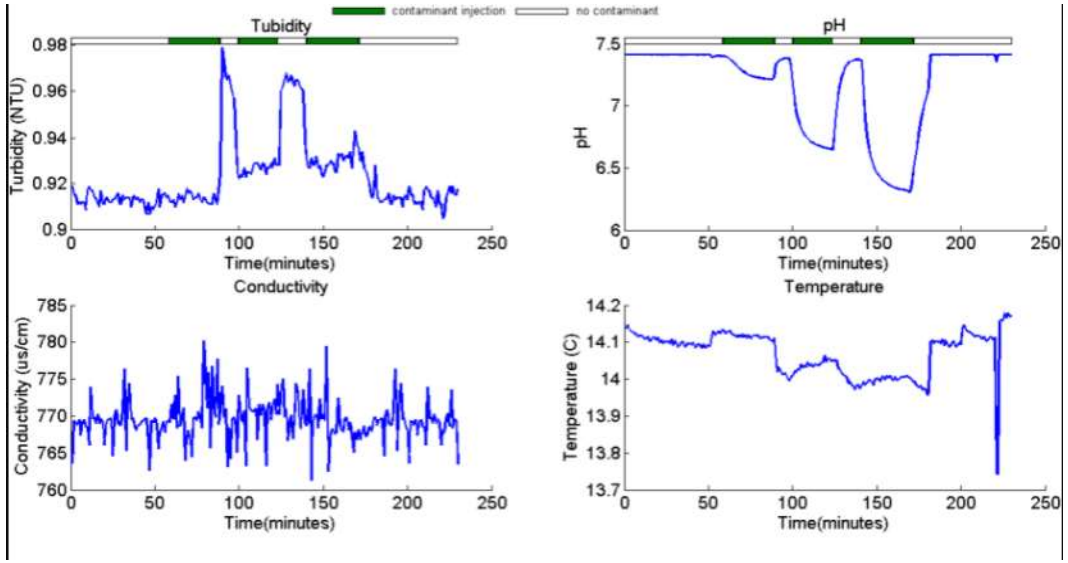
Ejeian et al. (2018), https://doi.org/10.1016/j.bios.2018.07.019

Biosensors


Pros
High sensitivity to biological contaminants
Suitable for in-situ monitoring
Minimum sample preparations
Portable and miniaturization
Fast response time
Effect-based system
Able to detect emerging contaminants
Sensitive to environment
Lack of system stability
Limited transducer life expand
Risk of bio-receptor leakages
Cons

Sensor placements approach

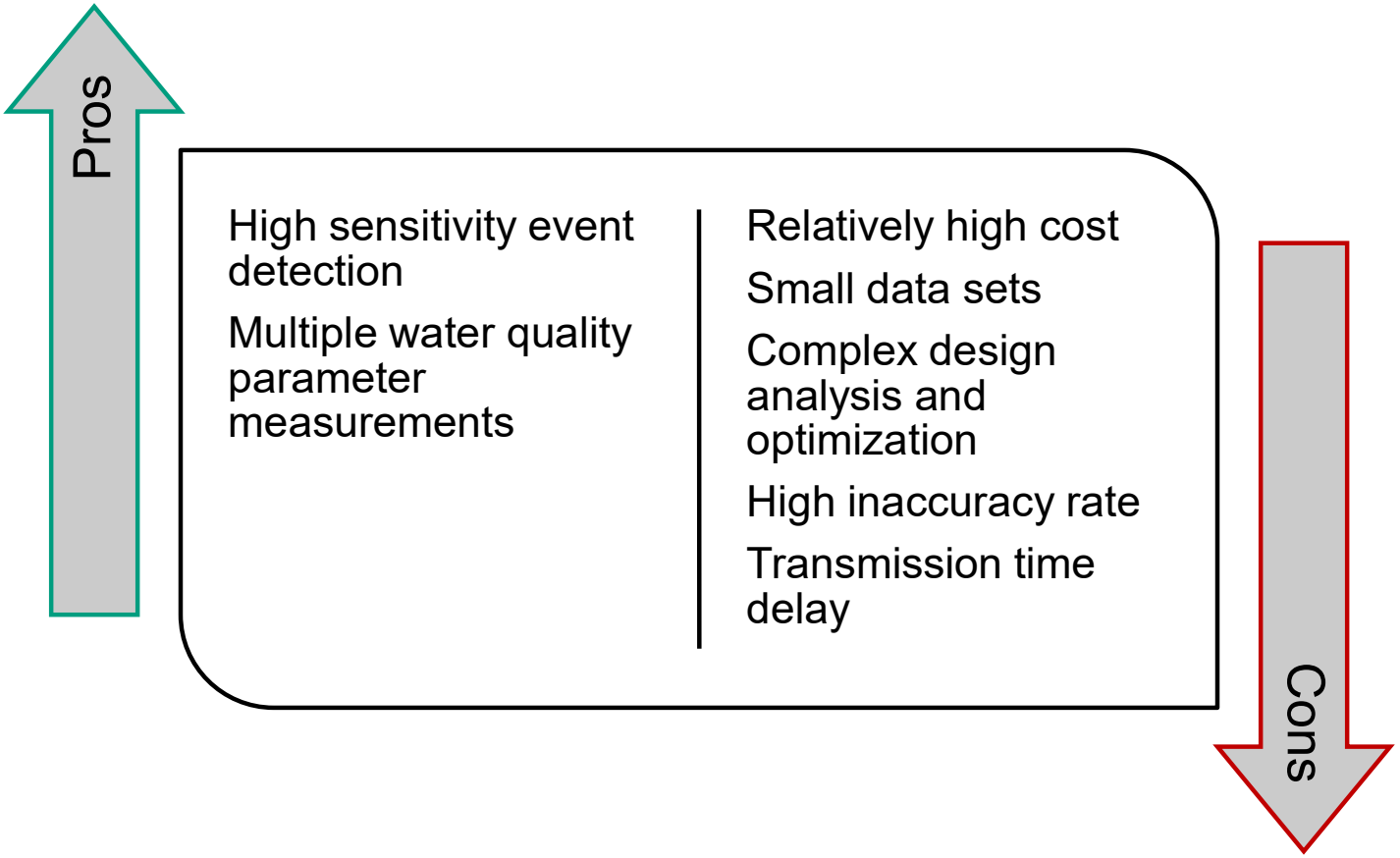




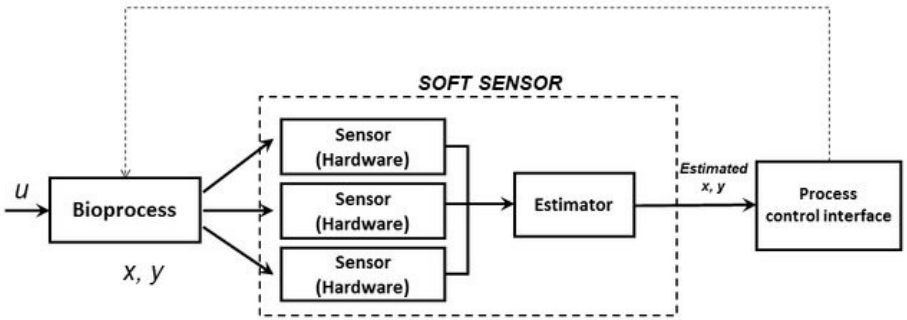
Sensor responses (Turbidity, pH, Conductivity and Temperature) for glyphosate (concentrations: 0.8, 2.0, 4.0 mg/L)

Che et al. (2015), https://doi.org/10.3390/w7041422

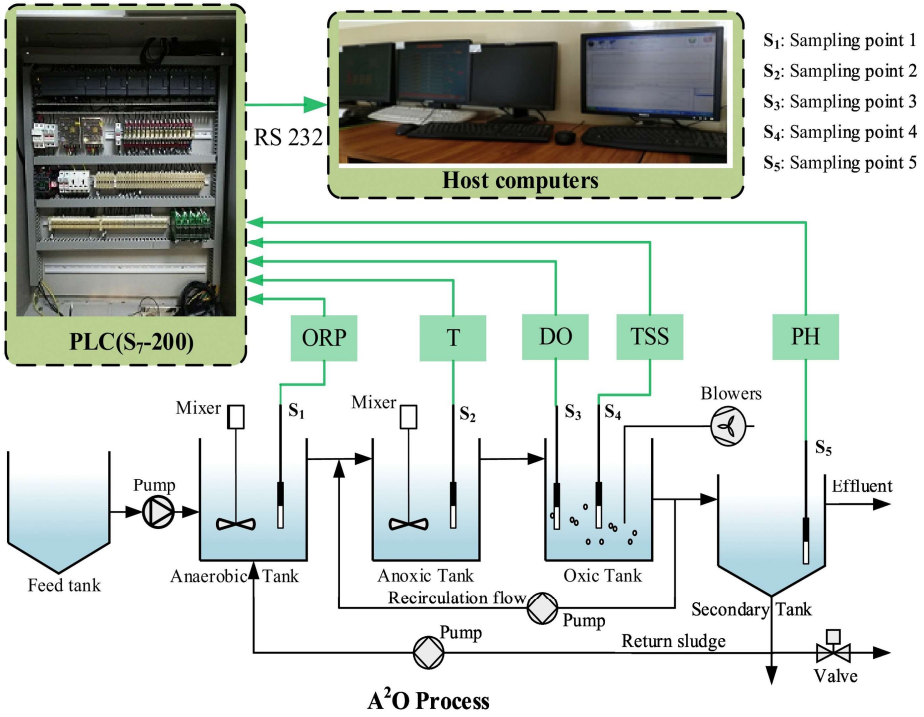
Sensor placements approach



Data-driven soft(ware) sensors



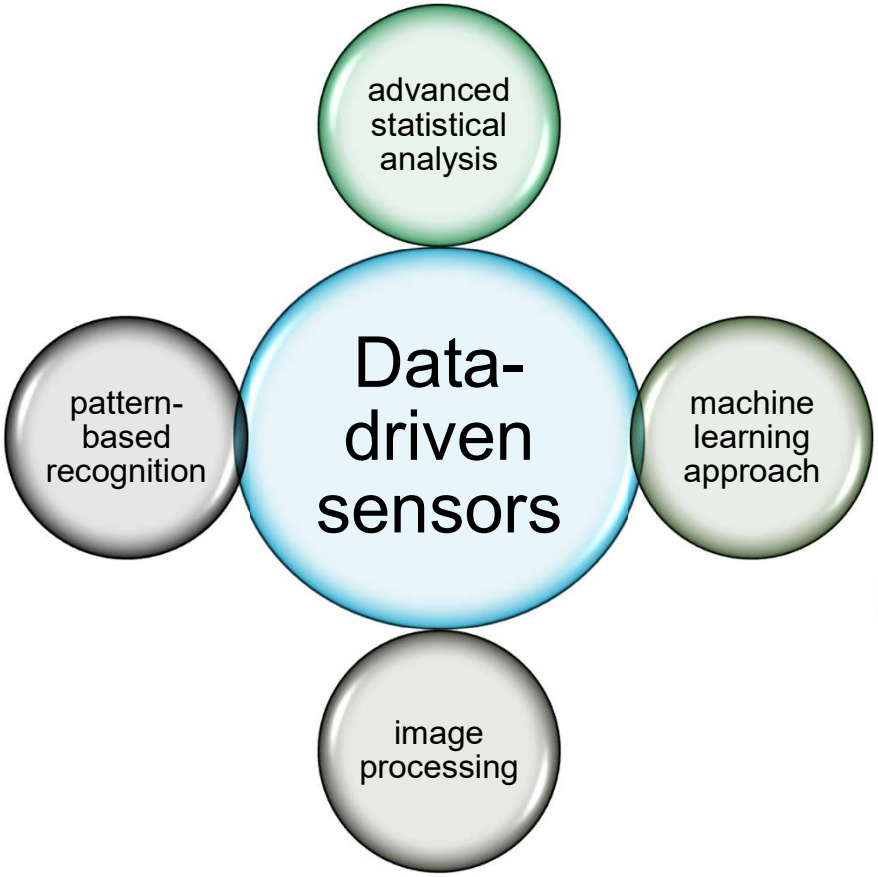
Soft sensor principle

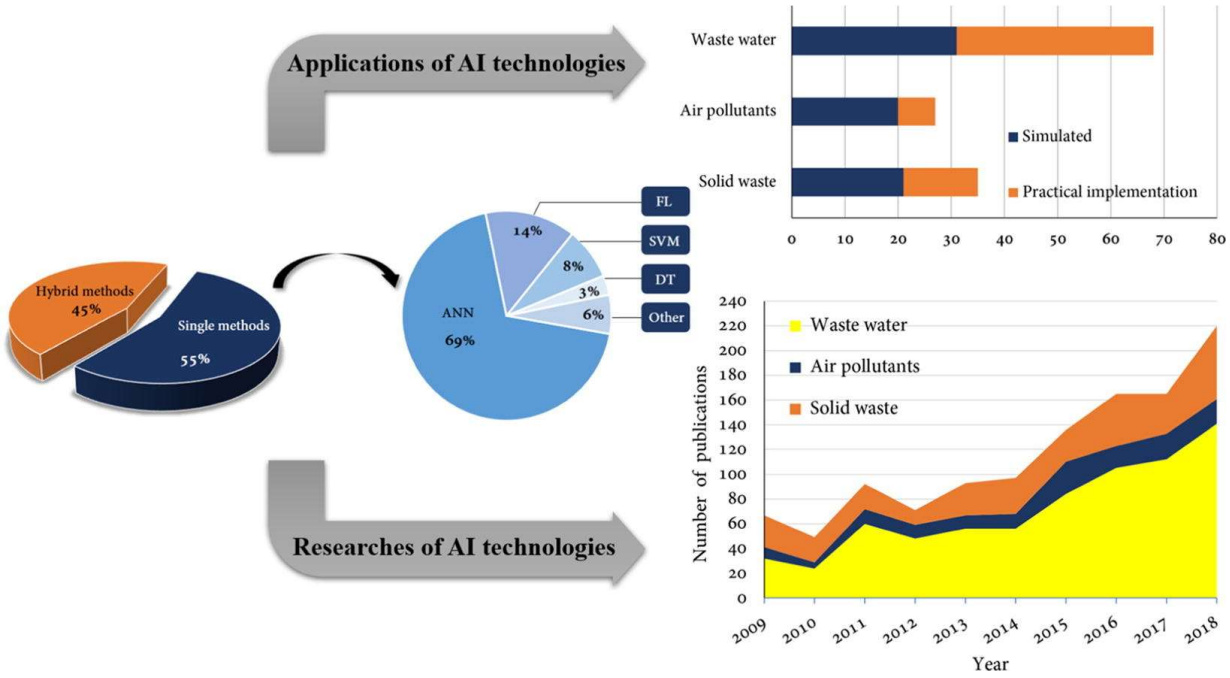


Monitoring system of total phosphorous and ammonia nitrogen concentrations in effluent

Norwegian University of Life Sciences

Paulsson et al. (2014), https://doi.org/10.3390/s141017864
Han et al. (2018), https://doi.org/10.1016/j.cjche.2018.03.027





Ye et al. (2020), https://doi.org/10.1016/j.scitotenv.2019.134279

AI models and machine learning algorithms in wastewater treatment

Pollutant removal processes

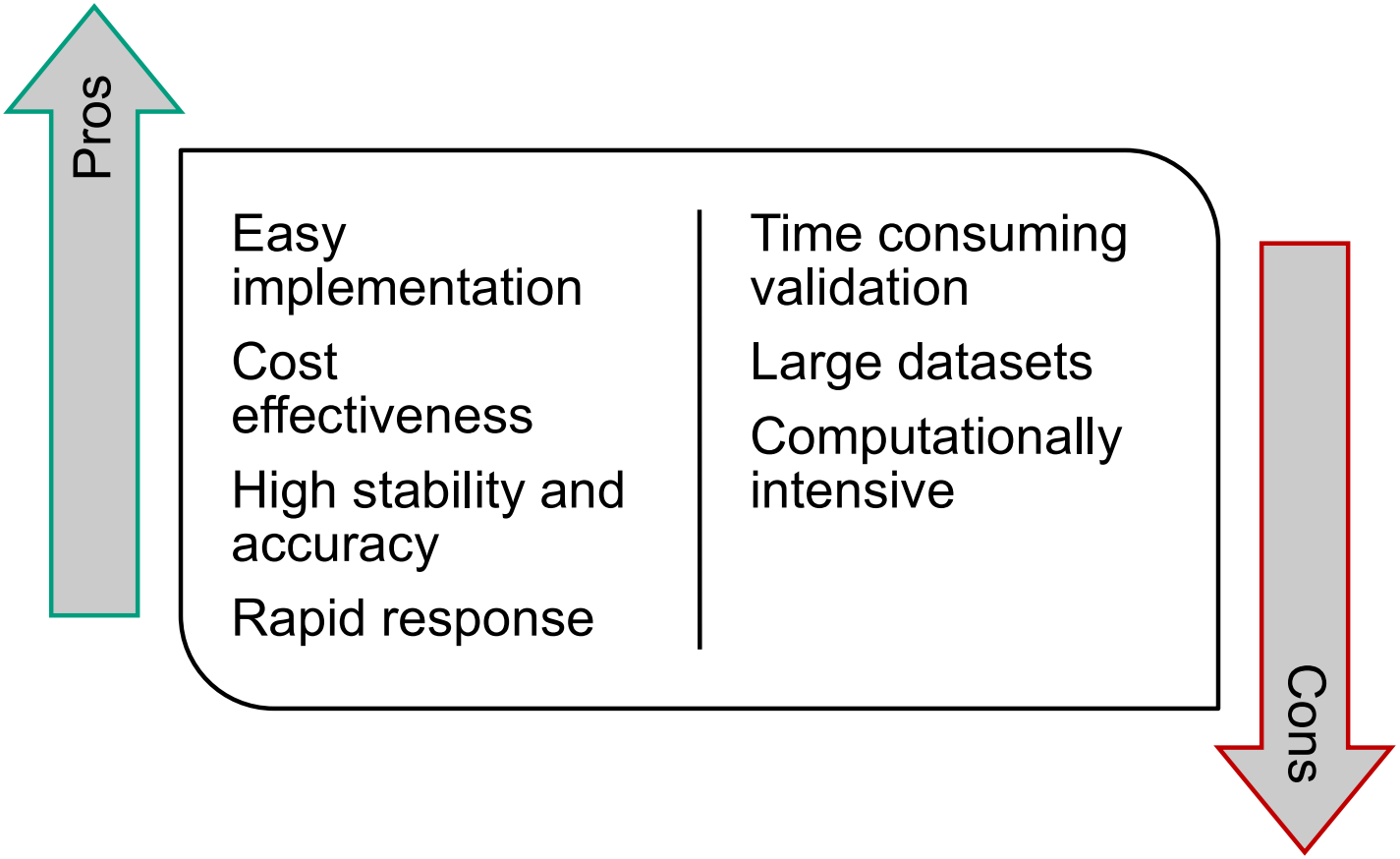
Heavy metals	Phosphate
COD	Color
Sulfate ions	Chlorophenol, naphtalene, triamterene

Processes control

Effluent coliform counts	Nitrate and ammonia concentration
Oxidation-Reduction Potential	DO, TSS, TDP, TSP
Effluent COD	Naphthalene removal efficiency

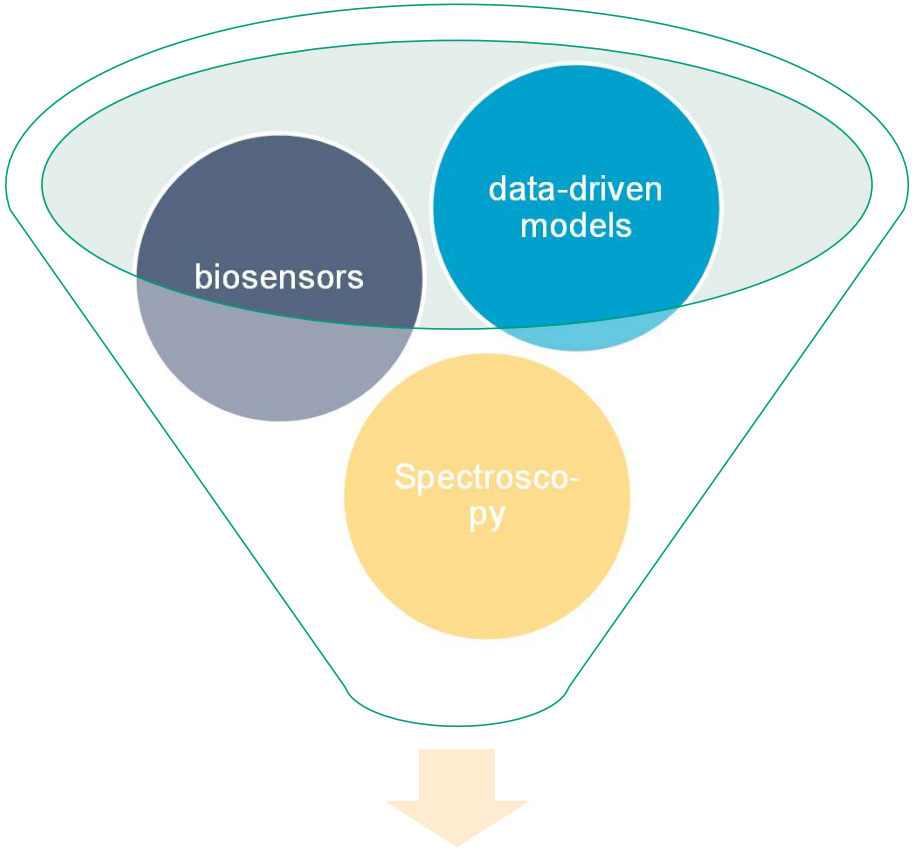
Ye et al. (2020), https://doi.org/10.1016/j.scitotenv.2019.134279

AI models and machine learning algorithms



HORIZON 2020

Development of Emerging Contaminants – Hybrid Soft Sensor for on-line monitoring of contaminants of emerging concern in water



Hybrid sensor

Thank you!