



Emerging Pollutants: Protecting Water Quality for the Health of People and the Environment

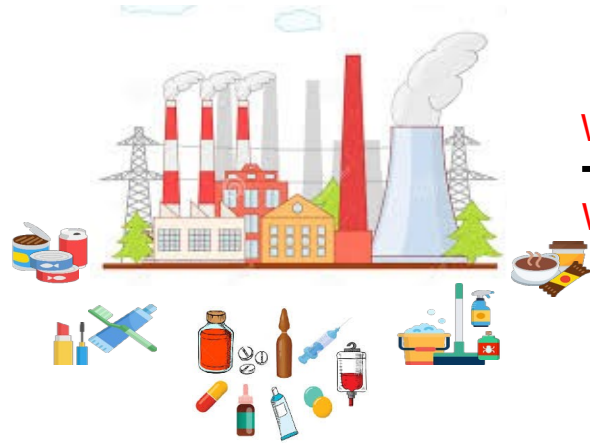
**Water contamination in a multi-industrial region in Brazil:
Decision support for water quality evaluation and
management of contaminants of emerging concern.**

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Fernando C.G. Murga, Fernando.F.Sodré.**

17th January 2023/ 15:55 CET



Industrial development *versus* environmental health.. Is the scale balanced?



WWTP-M = 23 kg of CEC/dia

WWTP-I = 115 kg of CEC/dia



Developing countries:





➤ **2018** largest and one of the largest in the country

➤ **Primary treatment.**

➤ **1st in Latin America.**

➤ **Reports on non-compliance with legislation**

Occurrence of CEC? WHICH ONES?

POLOCENTRO 2A ETAPA

POLOCENTRO 1A ETAPA

POLOCENTRO L

SÃO JOÃO

RES. MARIA CRISTINA

VILA ESPERANÇA

JARDIM SÃO PAULO

UEG Câmpus Henrique Santillo

Rio da Estrema

Rio dos Antas

ROQUE PA

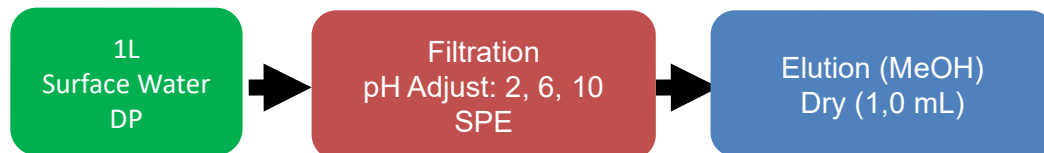
DP


WWTP

DISTRITO AGROINDUSTRIAL DE ANÁPOLIS

DAIA

Which ones? how much?

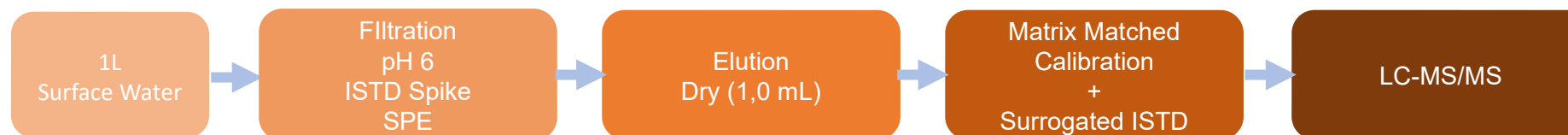


- High Resolution Mass Spectrometry
- Spectrum Data Base: 

Fosinopril, sulphapyridine, erlotinib, tropisetron



Triple TOF 5600+, Sciex



$mLOQ = 2,5 \text{ ng/L}$

mLOQ Level

Replicates

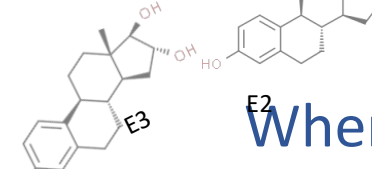
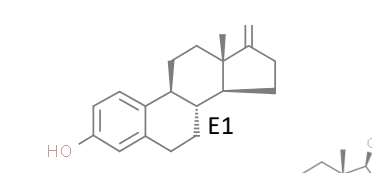
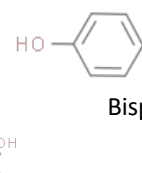
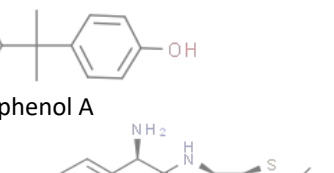
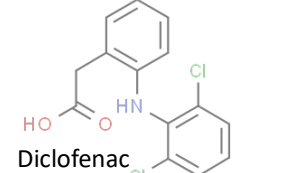
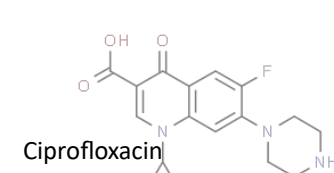
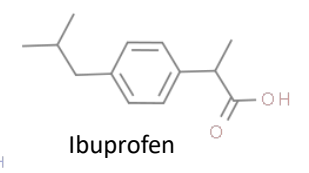
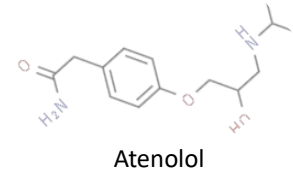
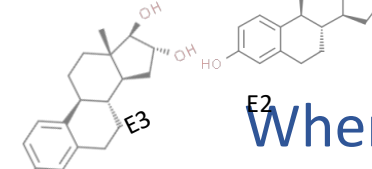
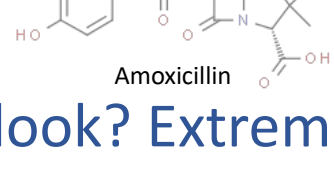
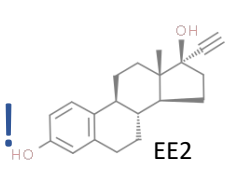
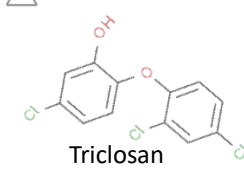
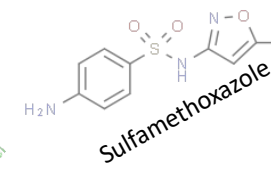
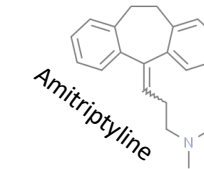
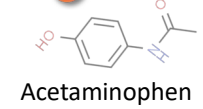
$CV \leq 17 \%$

Samples

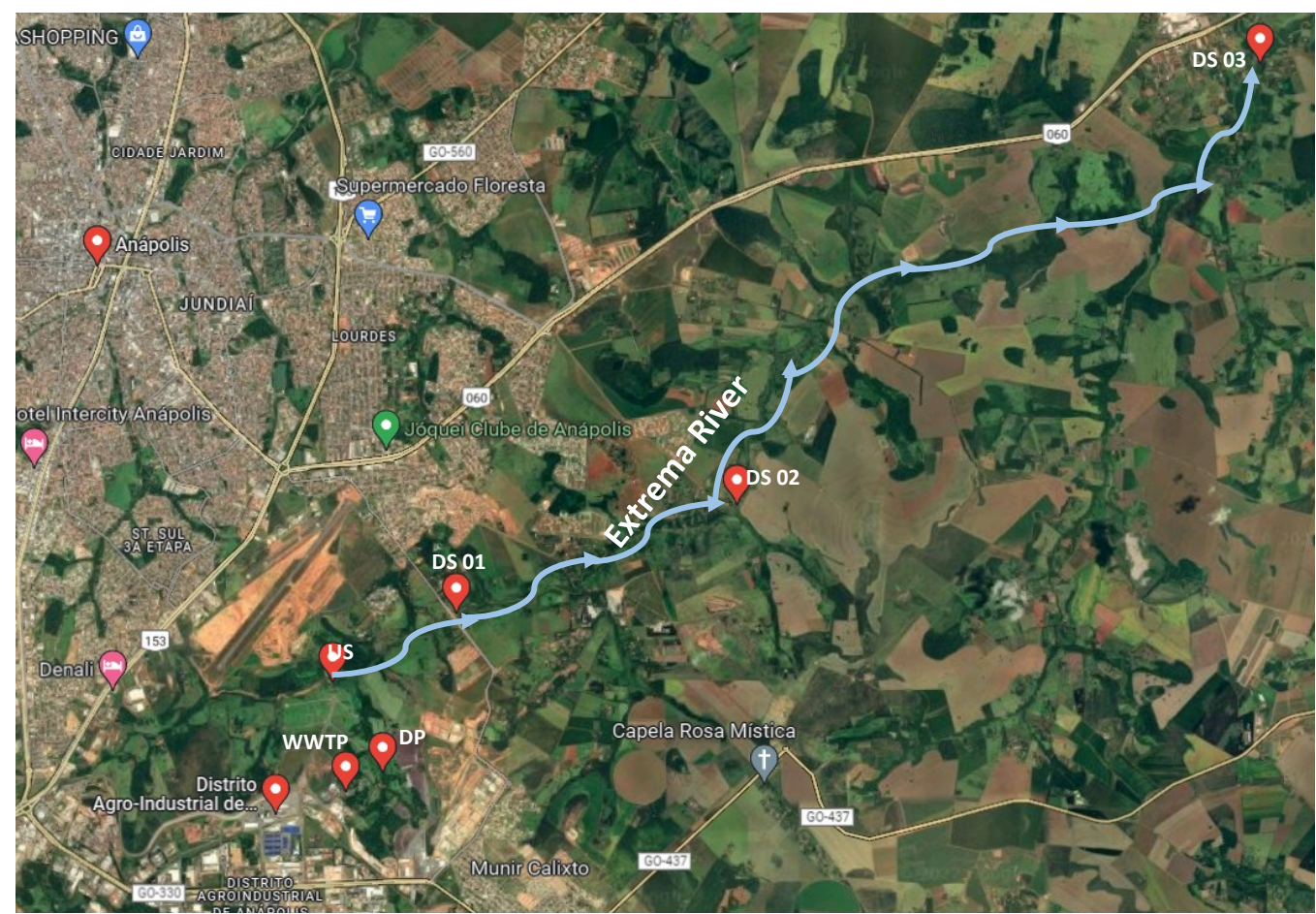
$mLOD = 0,75 \text{ ng/L}$



QTRAP 3200, Sciex



Where to look? Extrema River!



Upstream (US)



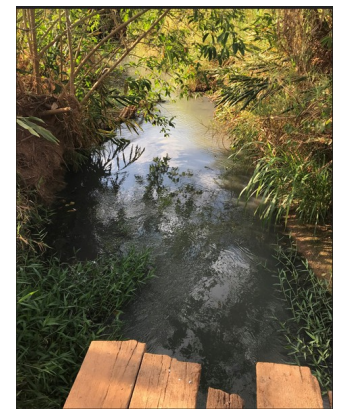
Discharge Point (DP)



Downstream 01 (DS01)



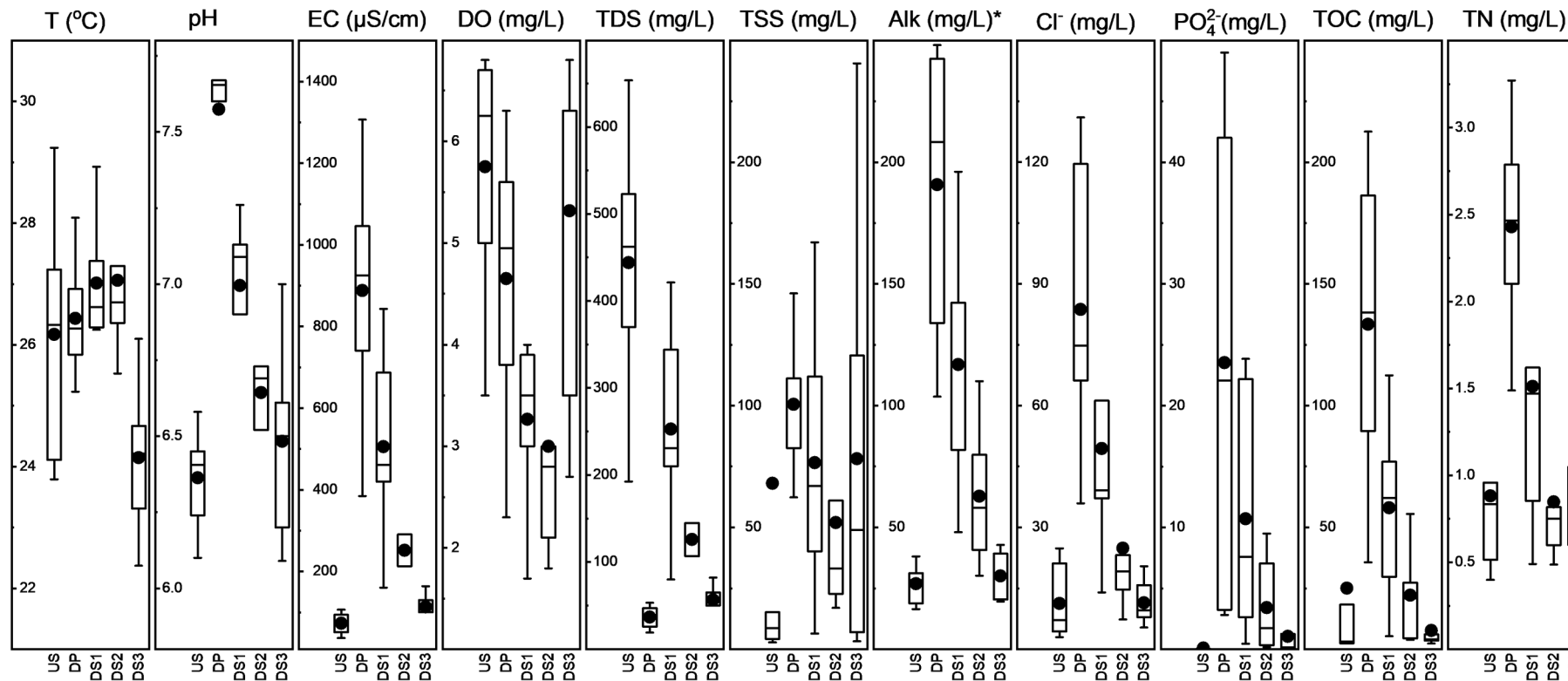
Downstream 02 (DS02)



Downstream 03 (DS03)



Other Parameters considered: CONAMA 357/2008



*in dissolved fraction, lotic environment.

CEC concentration: how much risk?

- Concentration Range:
 - $3,5 \pm 0,3$ ng/L e $11,7 \pm 0,1$ µg/L
- Daily Load:
 - Brazil: 551 g.dia⁻¹
 - Spain: $29,4$ g.dia⁻¹

Risk Assessment:

$$RQ = \frac{MEC}{PNEC}$$

DPS, CFX, BPP, TEO, DIA,
 BZF, HCT, CHO

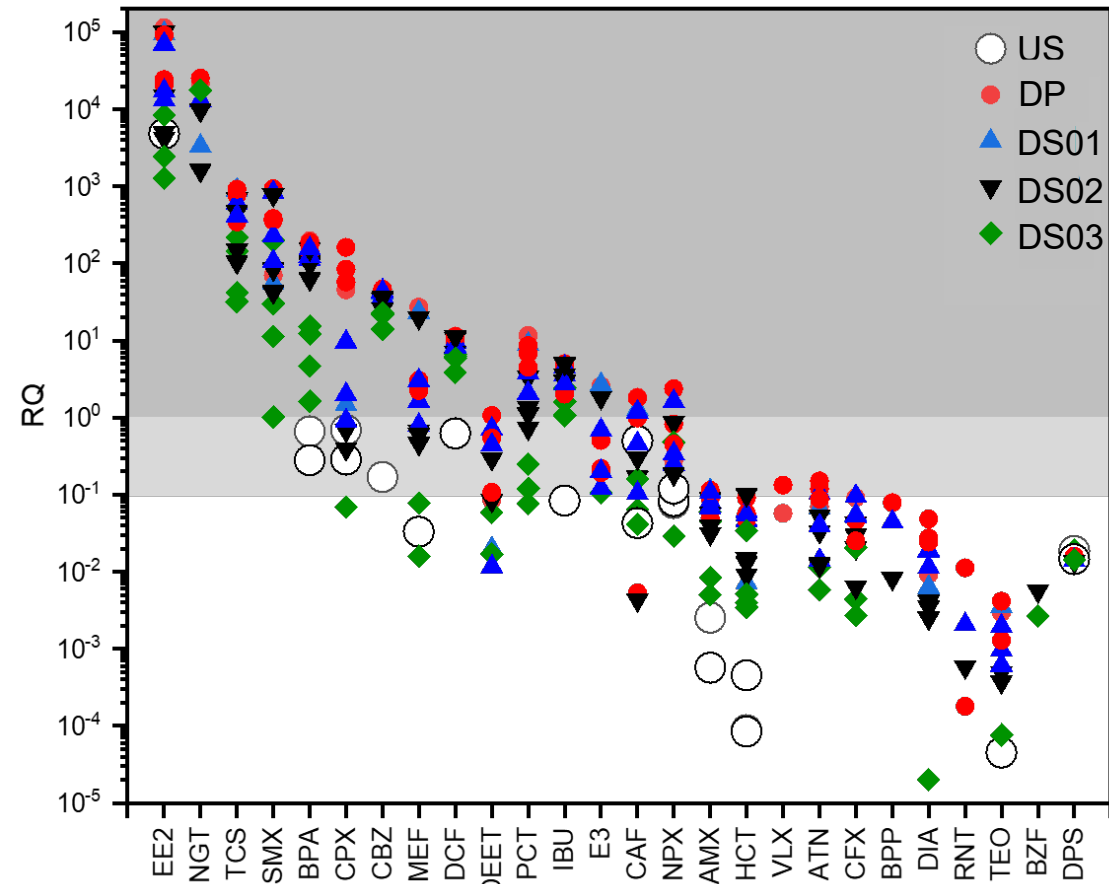
↓ [] ↑ PNEC

ATN, VLX, AMX,
 CAF, NPX

↑ [] ↑ PNEC

SMX, CBZ, TCS, EE2, NGT, BPA,
 IBU e DCF

↑ [] ↓ PNEC



A broader approach: WQI Canadian Council of Ministers for the Environment

- Flexible algorithm
- Allows you to select policy values!

WQI-CCME range	Water Quality
100 - 95	Excellent
94 - 80	Good
79 - 65	Fair
64 - 45	Marginal
44 - 0	Poor

Factor	Calculation
F1	
F2	
F3	<p>Step 1</p> <p>Step 2</p>

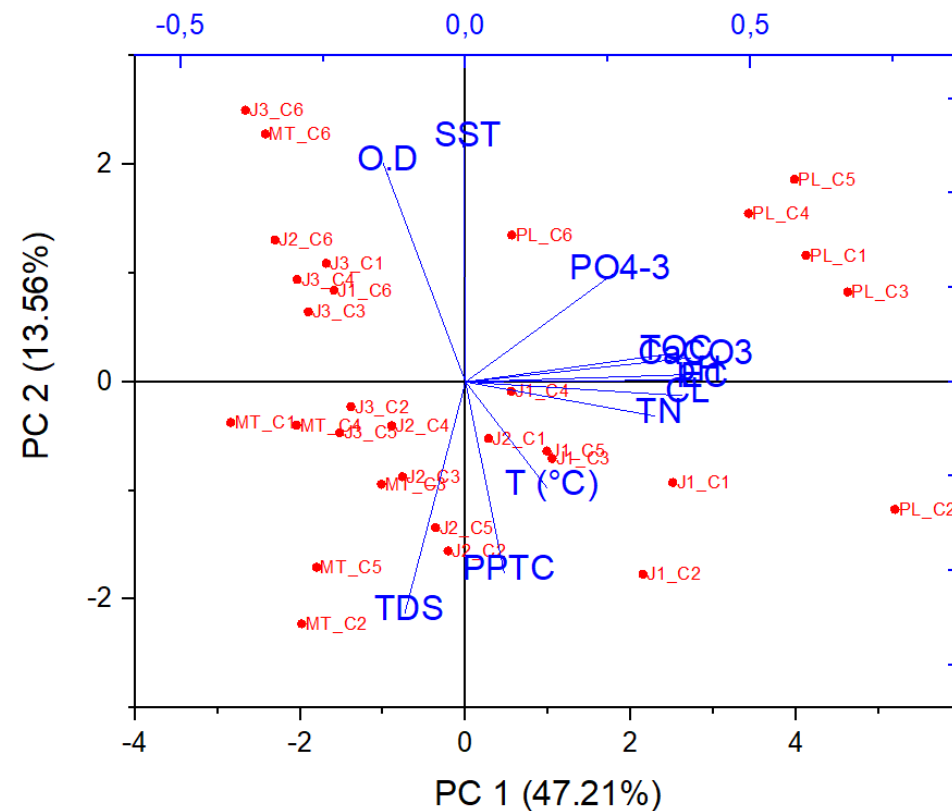
Adaptation: Water quality index per sampling point

➤ Variables F1 e F2 become equal!

- F1: Fault frequency
- F2: fault magnitude

➤ Variables that discriminate high and low quality

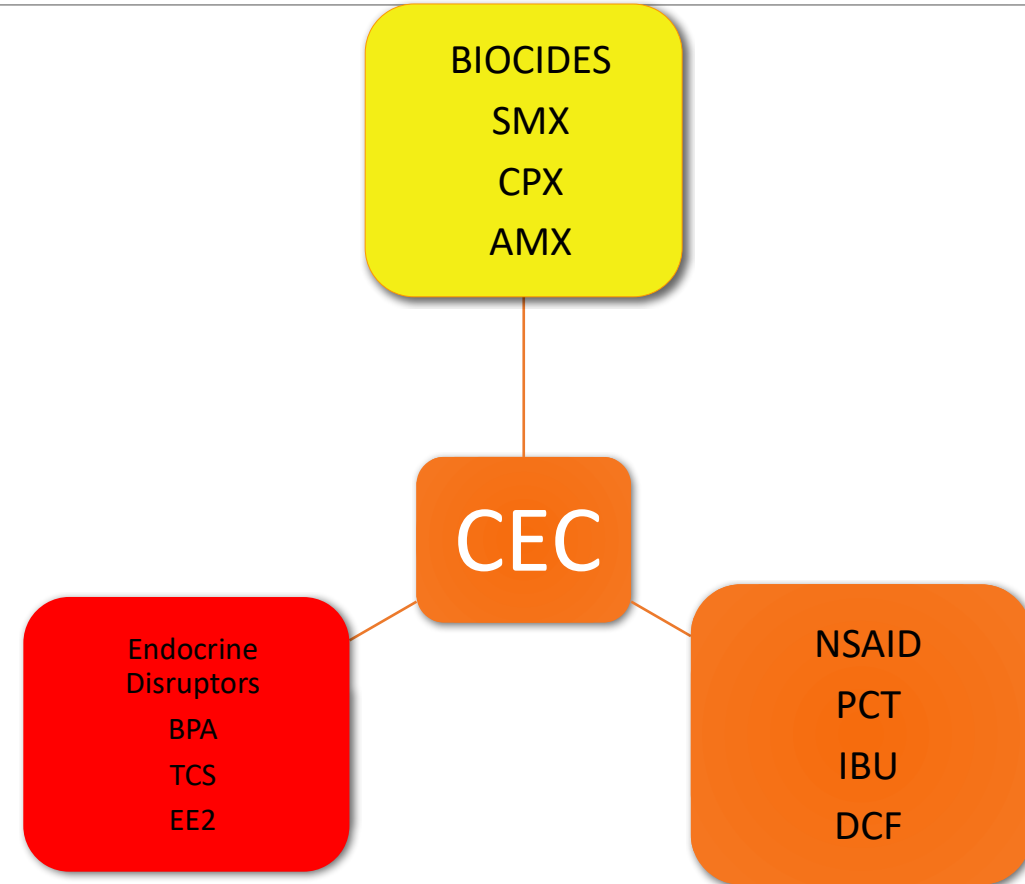
➤ Selected: EC, DO, PO₄³⁻ and TSS



Point	WQI -CCME	
	All Parameters	After PCA
US_C1	87	100
DP_C1	61	47
DS 01_C1	61	29
DS 02_C1	68	47
DS 03_C1	87	82
US_C2	81	100
DP_C2	55	29
DS 01_C2	61	29
DS 02_C2	68	47
DS 03_C2	74	47
US_C3	81	82
DP_C3	61	29
DS 01_C3	68	47
DS 02_C3	68	47
DS 03_C3	74	65
US_C4	94	100
DP_C4	61	29
DS 01_C4	61	29
DS 02_C4	68	47
DS 03_C4	74	65

Concerning CEC: How to include them?

- CEC are barely included in routine WQ analysis
- CEC pose threat to aquatic life
- Include CEC in adapted WQIs
- Candidate Lists
- PNECs as guidelines



As a result...

- More restrictive quality index values when including CEC

- Almost all WQIs from DP to DS3 are considered poor

- Adapted WQICCMs indicate a scenario more consistent with local pollution

Point	WQI -CCME	
	After PCA	Including EMP
US_C1	100	95
DP_C1	47	12
DS 01_C1	29	14
DS 02_C1	47	21
DS 03_C1	82	54
US_C2	100	94
DP_C2	29	15
DS 01_C2	29	20
DS 02_C2	47	39
DS 03_C2	47	44
US_C3	82	95
DP_C3	29	28
DS 01_C3	47	34
DS 02_C3	47	39
DS 03_C3	65	49
US_C4	100	100
DP_C4	29	28
DS 01_C4	29	34
DS 02_C4	47	44
DS 03_C4	65	49

Finally

- Total concentrations of CECs were more than ten times higher compared to receiving waters impacted by municipal wastewater discharges
- First glimpse of potential risks caused by CECs from industrial sources in Brazil
- A simple and comprehensive estimate for water quality was proposed to guide decision making

Thank you

