



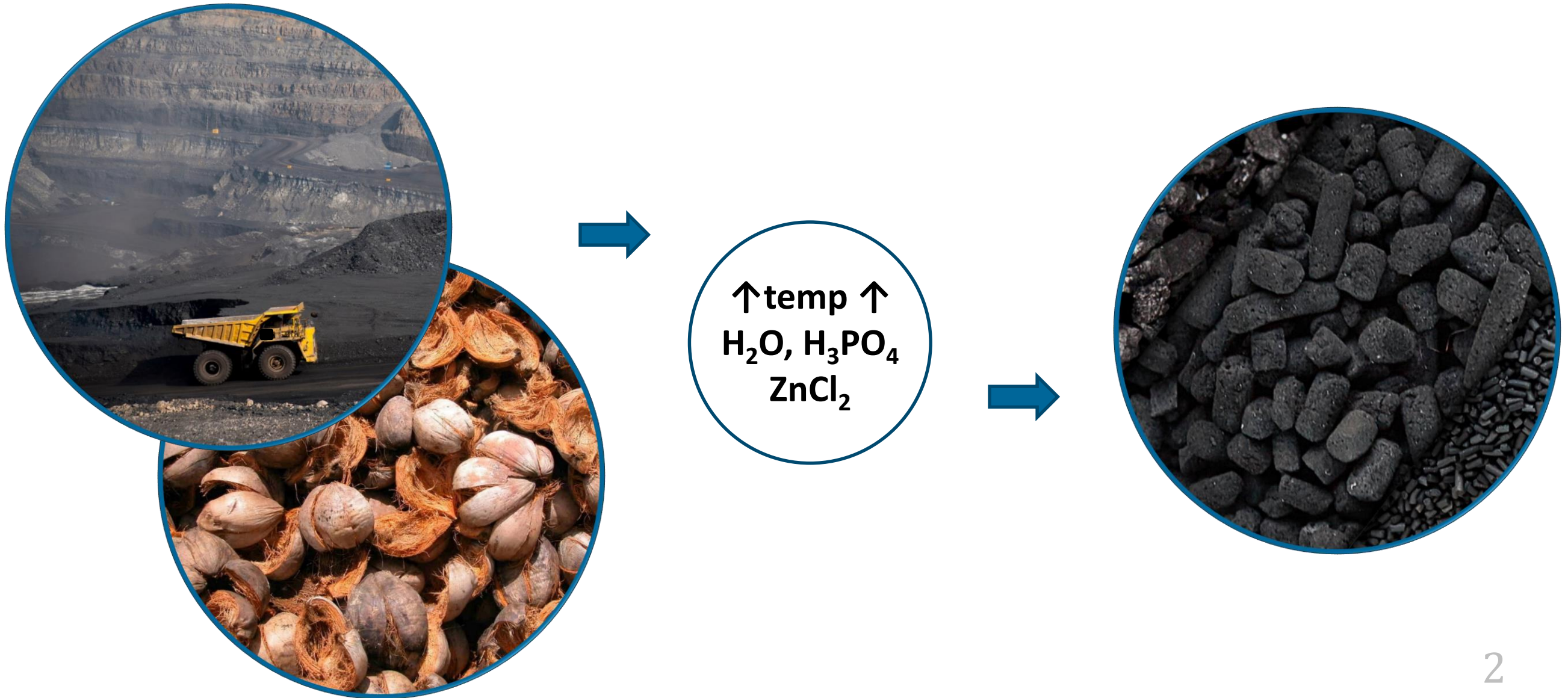
universität  
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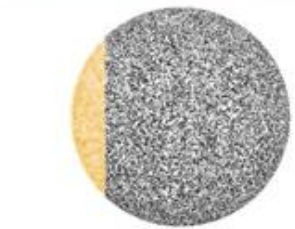
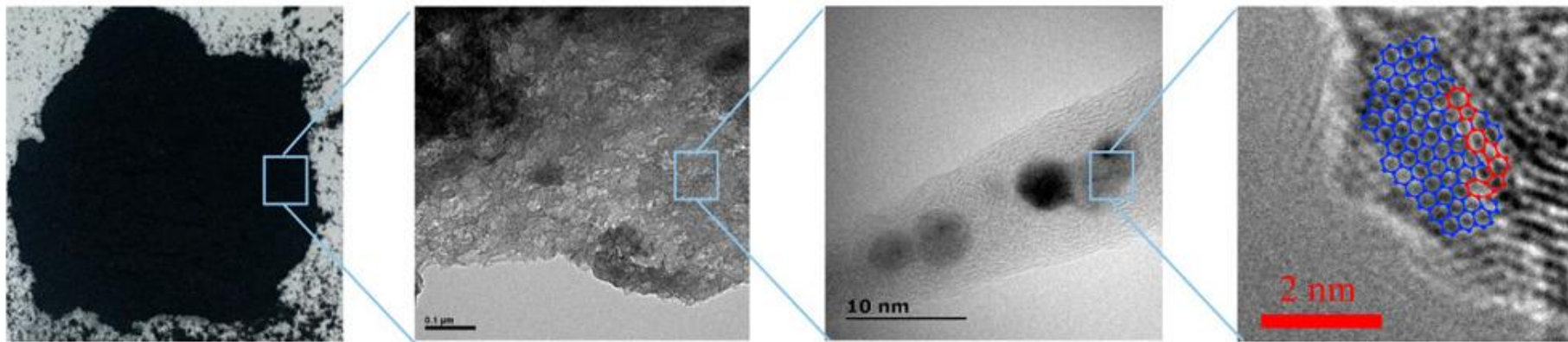
# **A critical perspective on activated carbon for the removal of PMTs/vPvMs from aqueous solutions**

[gabriel.sigmund@univie.ac.at](mailto:gabriel.sigmund@univie.ac.at)

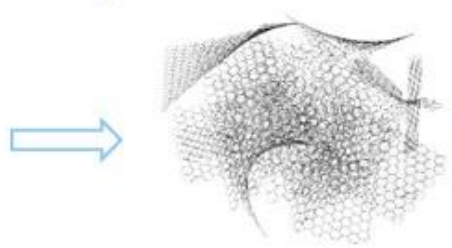
# What is activated carbon?



# How does activated carbon work?



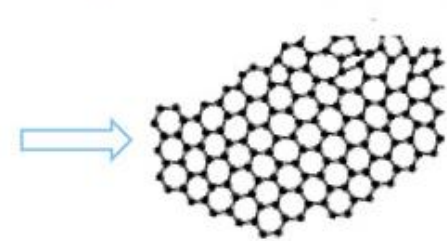
Heterogeneous phases



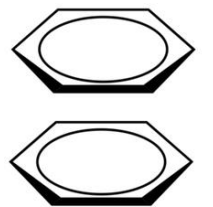
Graphene-like aggregates



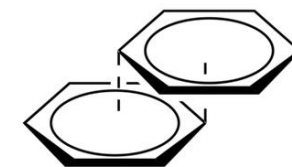
Aromatic clusters



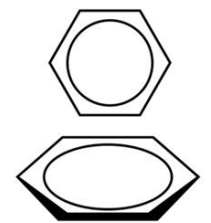
Atomic arrangement



sandwich



displaced



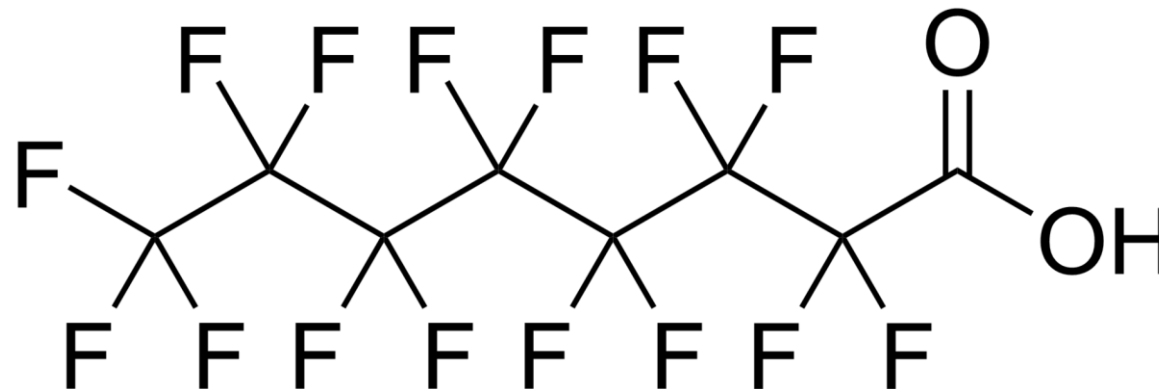
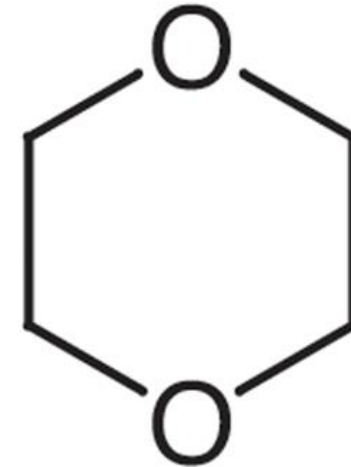
edge-to-face

<https://doi.org/10.1021/acs.est.6b06300>

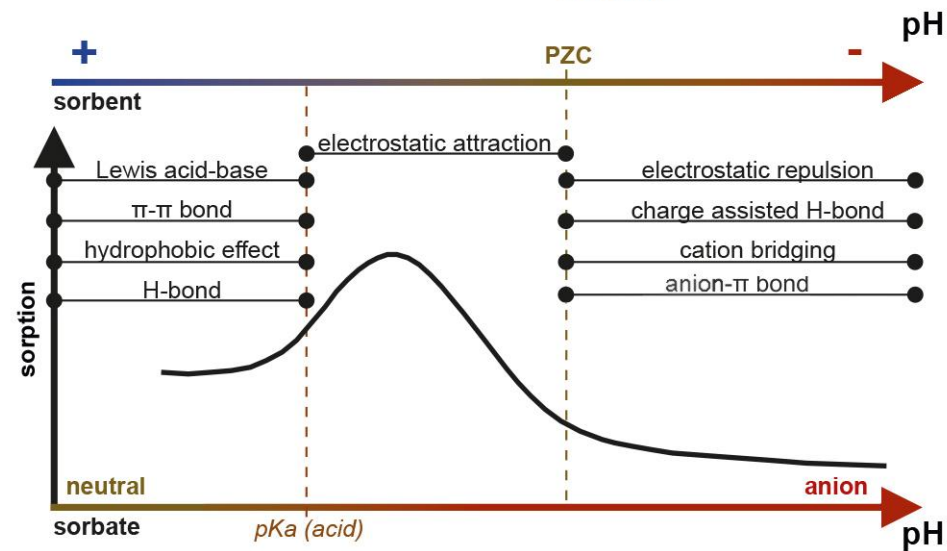
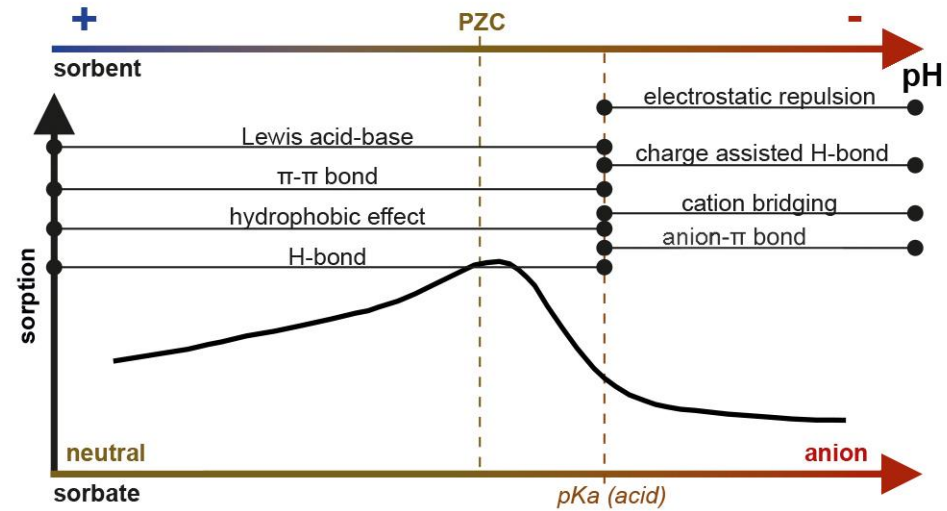
# What about PMT / vPvM substances?

## PMT / vPvM compounds in SIN list:

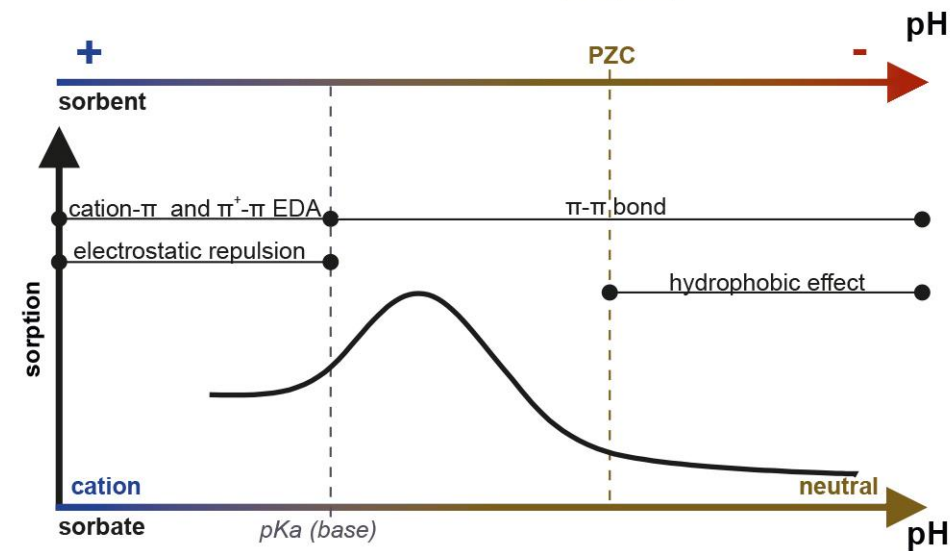
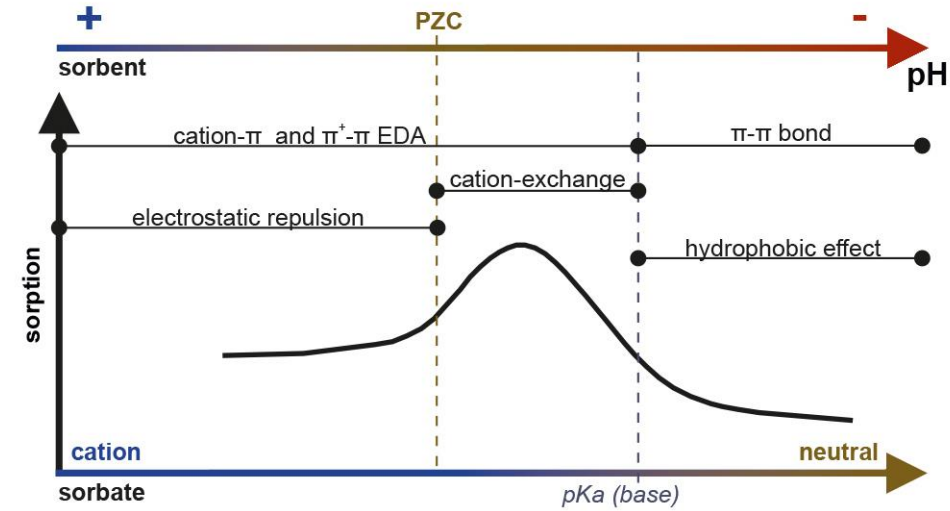
- 5 out of 34 are aromatic compounds
- 27 out of 34 are ionic/ionizable compounds



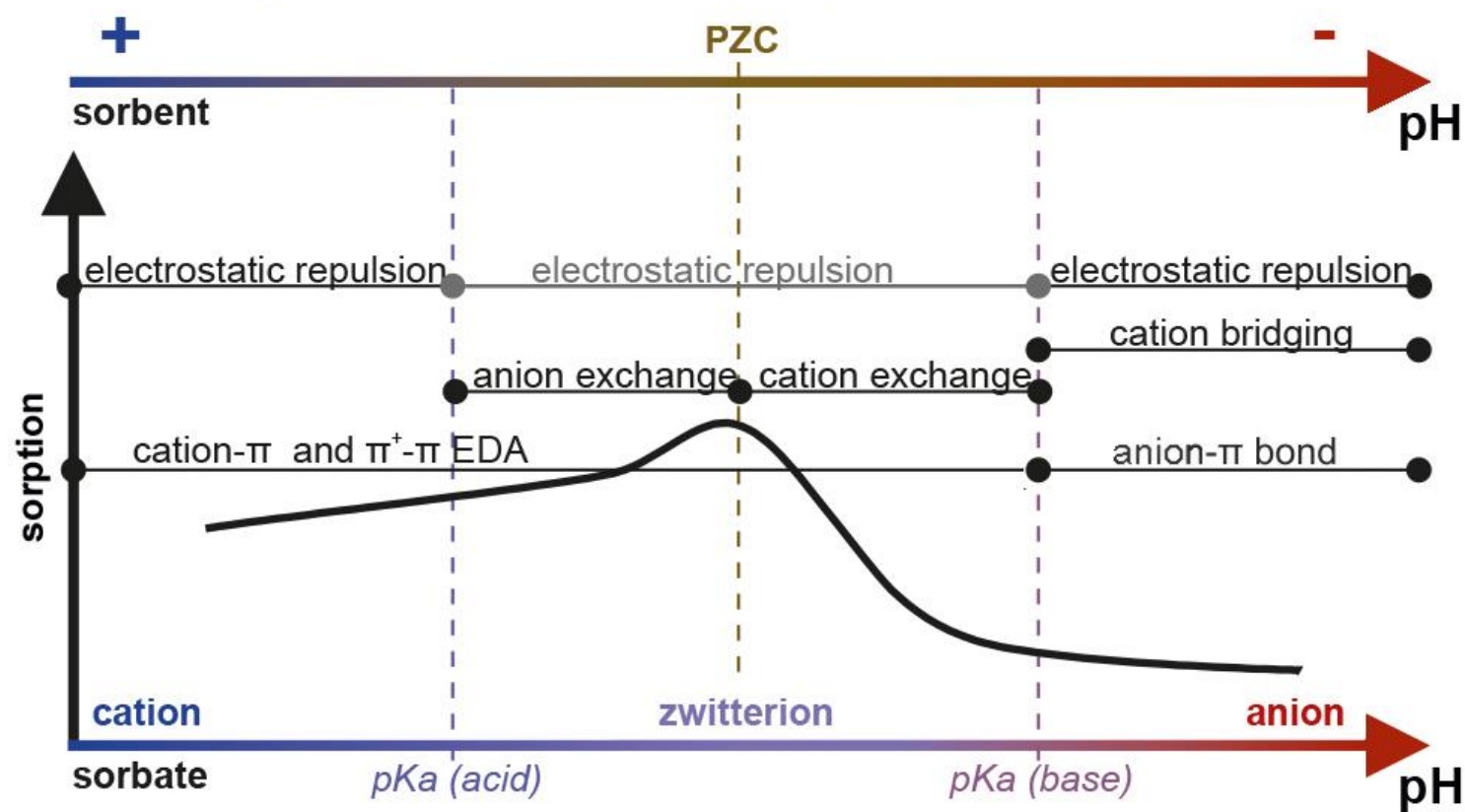
# Acids



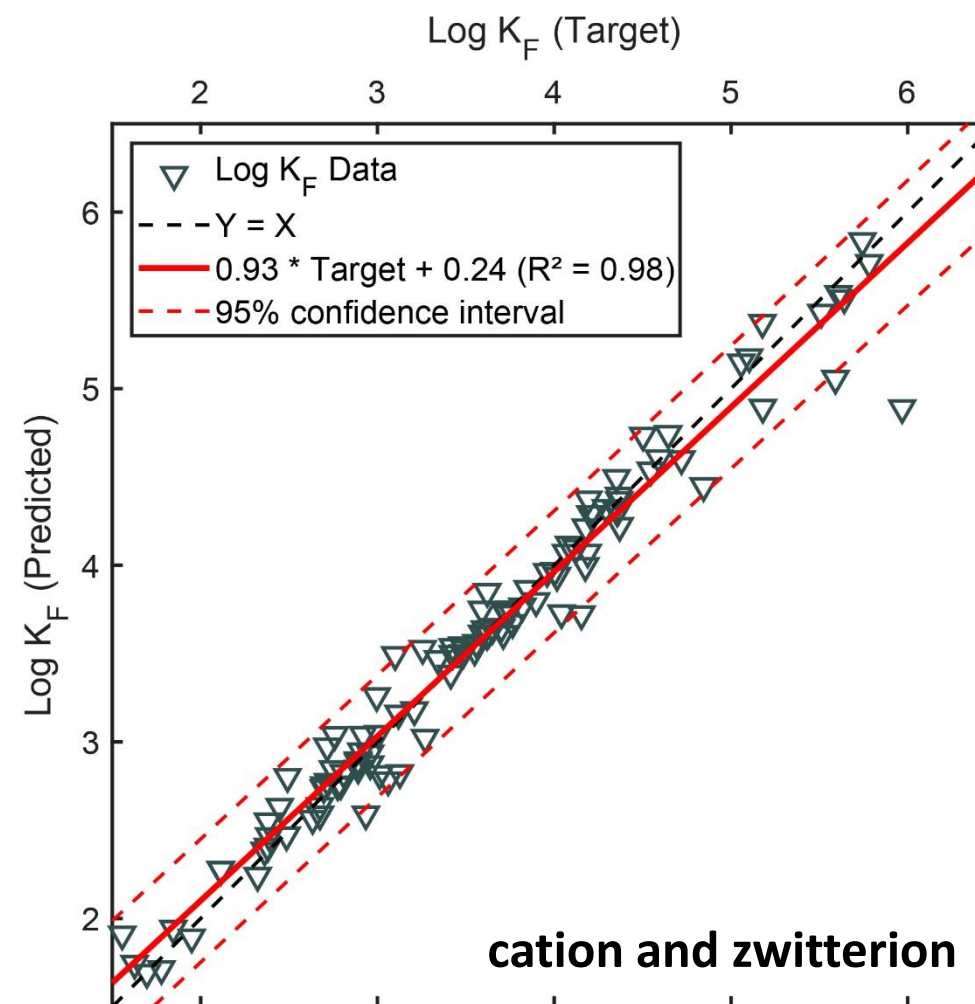
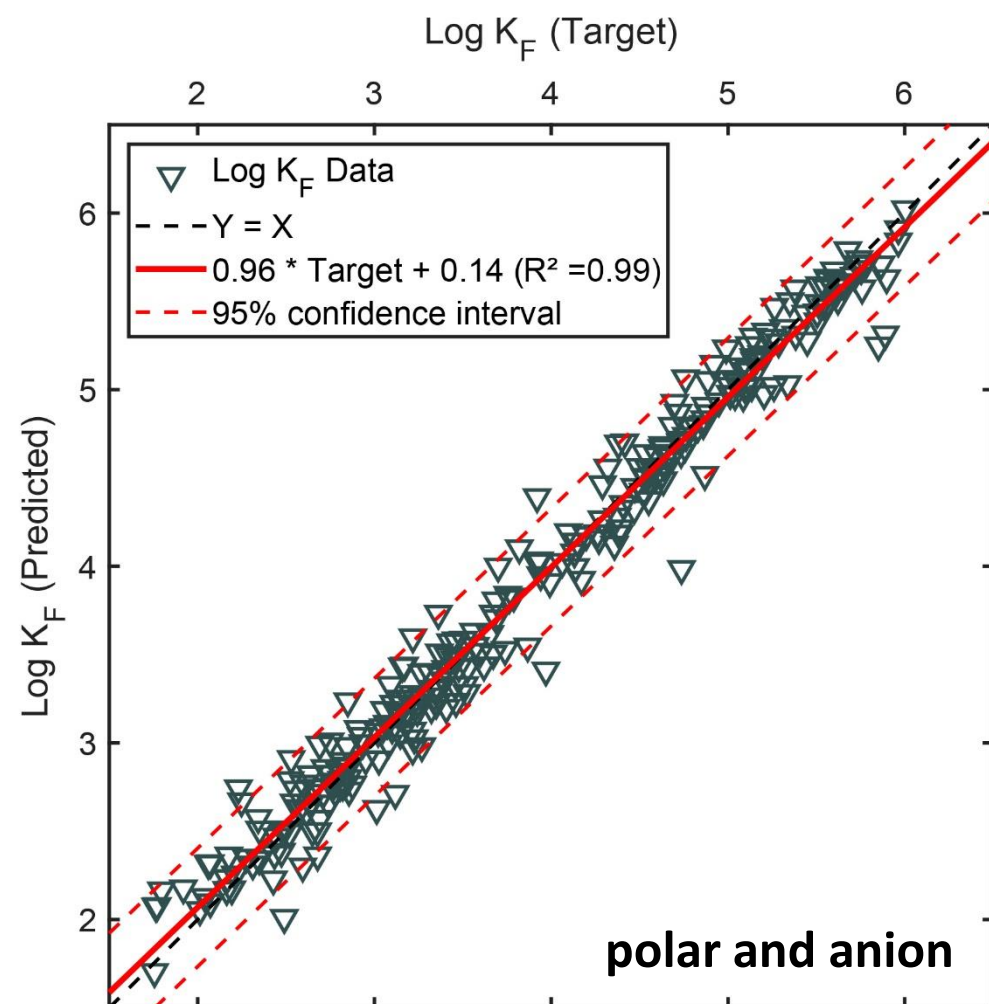
# Bases



# Amphoteric(Z)



# Is prediction possible?



# A practical (positive) example

anthropogenic organic  
micropollutants can be  
released to the natural  
environment via WWTPs

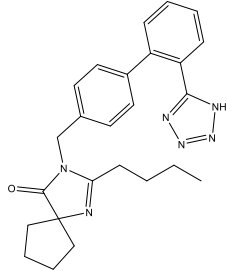
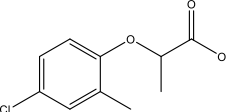
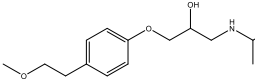
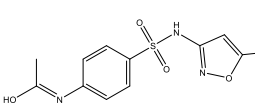
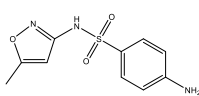
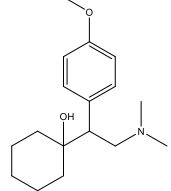


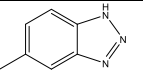
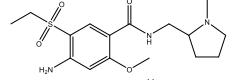
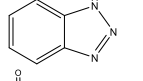
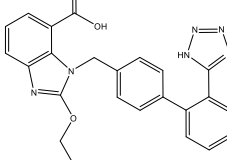
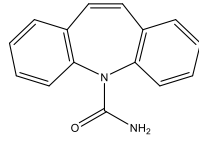
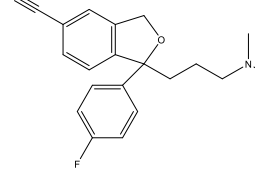
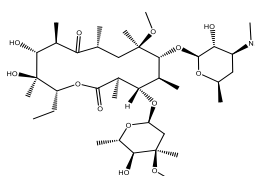
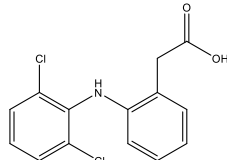
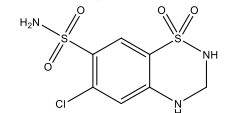
fourth purification stage



ebswien.at

# Micropollutants in WWTPs

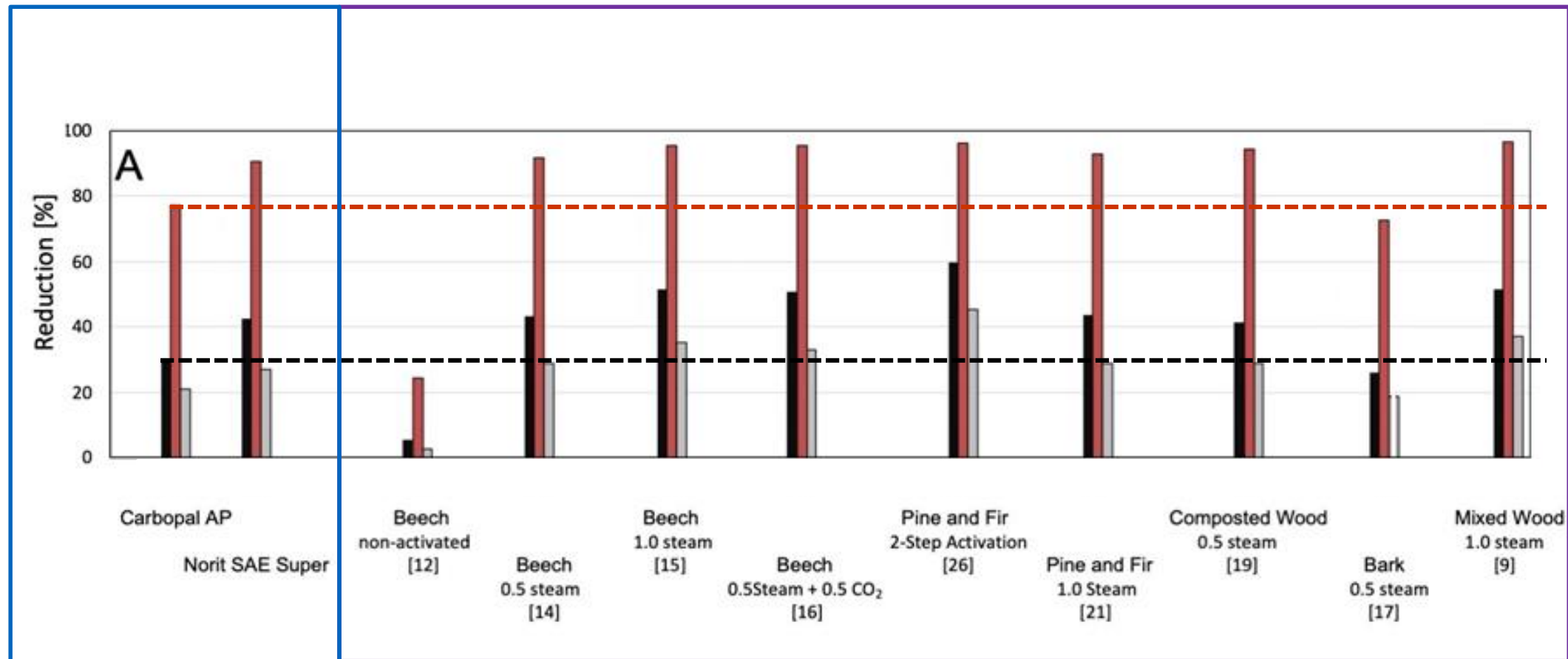
| compound                  | structure                                                                           | lowest pka         | pka base          | predominant species at pH 7.4 | Log D at pH 7.4 <sup>3</sup> |
|---------------------------|-------------------------------------------------------------------------------------|--------------------|-------------------|-------------------------------|------------------------------|
| Irbesartan                |    | 4.29 <sup>1</sup>  | 4.08 <sup>1</sup> | anion                         | 1.24                         |
| Mecoprop                  |   | 3.10 <sup>1</sup>  |                   | anion                         | -0.65                        |
| Metoprolol                |  | 14.00 <sup>1</sup> | 9.60 <sup>1</sup> | cation                        | -0.25                        |
| N4-Acetylsulfamethoxazole |  | 5.88 <sup>1</sup>  |                   | anion                         | -0.28                        |
| Sulfamethoxazole          |  | 5.70 <sup>1</sup>  | 1.70 <sup>1</sup> | anion                         | -0.56                        |
| Venlafaxin                |  |                    | 8.90 <sup>2</sup> | cation                        | 1.43                         |

| compound             | structure                                                                             | lowest pka         | pka base          | predominant species at pH 7.4 | Log D at pH 7.4 <sup>3</sup> |
|----------------------|---------------------------------------------------------------------------------------|--------------------|-------------------|-------------------------------|------------------------------|
| 5-Methylbenzotriazol |    | 9.12 <sup>2</sup>  | 0.45 <sup>2</sup> | neutral                       | 1.69                         |
| Amisulpride          |    | 13.20 <sup>2</sup> | 8.22 <sup>2</sup> | cation                        | -0.43                        |
| Benzotriazol         |    | 8.37 <sup>1</sup>  | 0.22 <sup>2</sup> | neutral                       | 1.5                          |
| Candesartan          |    | 3.50 <sup>1</sup>  | 2.45 <sup>1</sup> | anion                         | 0.04                         |
| Carbamazepin         |    |                    |                   | neutral                       | 2.45                         |
| Citalopram           |   |                    | 9.70 <sup>2</sup> | cation                        | 1.27                         |
| Clarithromycin       |  | 12.00 <sup>1</sup> | 8.99 <sup>1</sup> | cation                        | 2.38                         |
| Diclofenac           |  | 4.15               |                   | anion                         | 1.37                         |
| Hydrochlorothiazide  |  | 7.90 <sup>1</sup>  |                   | neutral                       | -0.01                        |

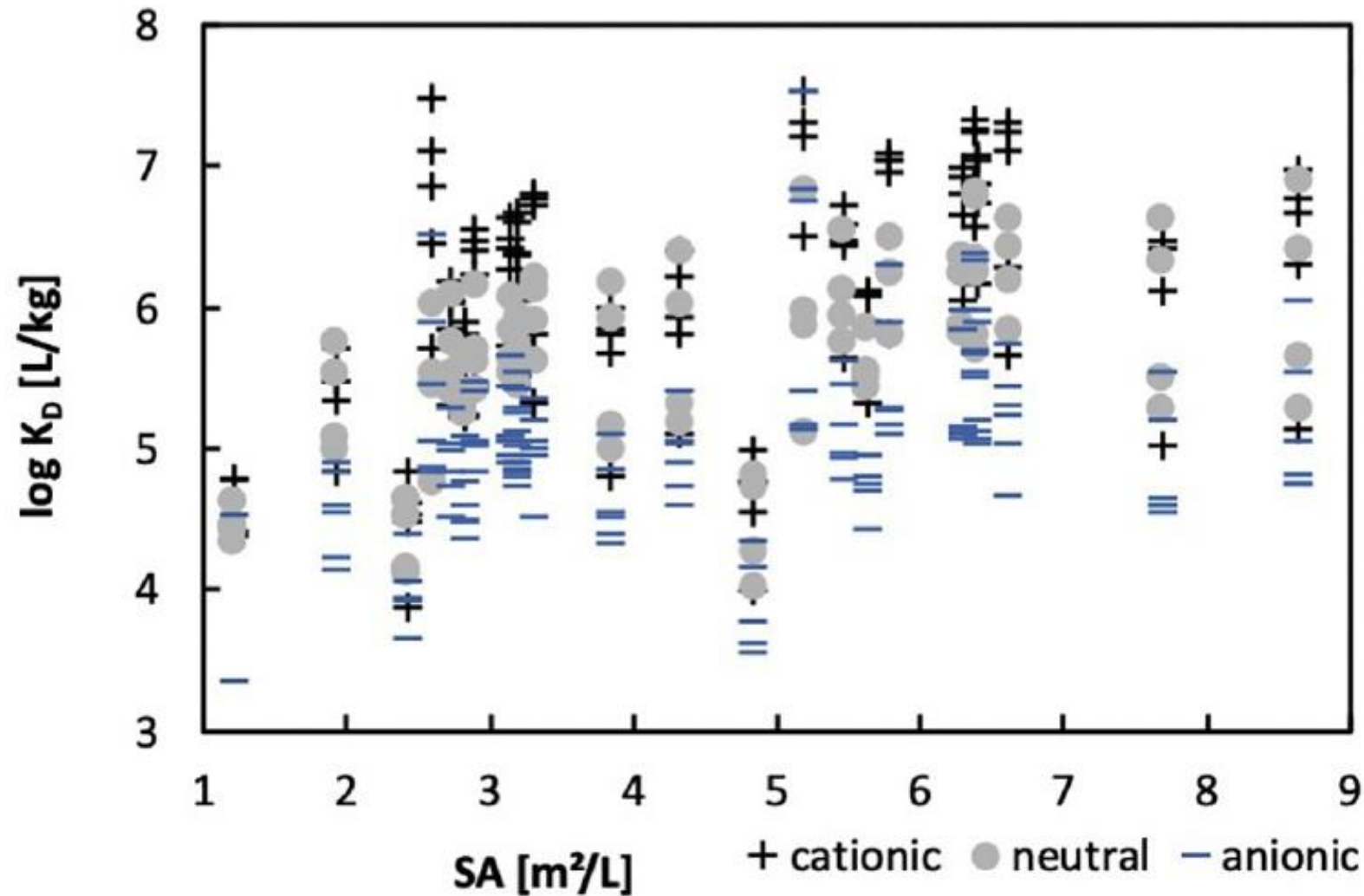
# Reduction of UV, DOC and OMP

Commercial

Wood based sorbents



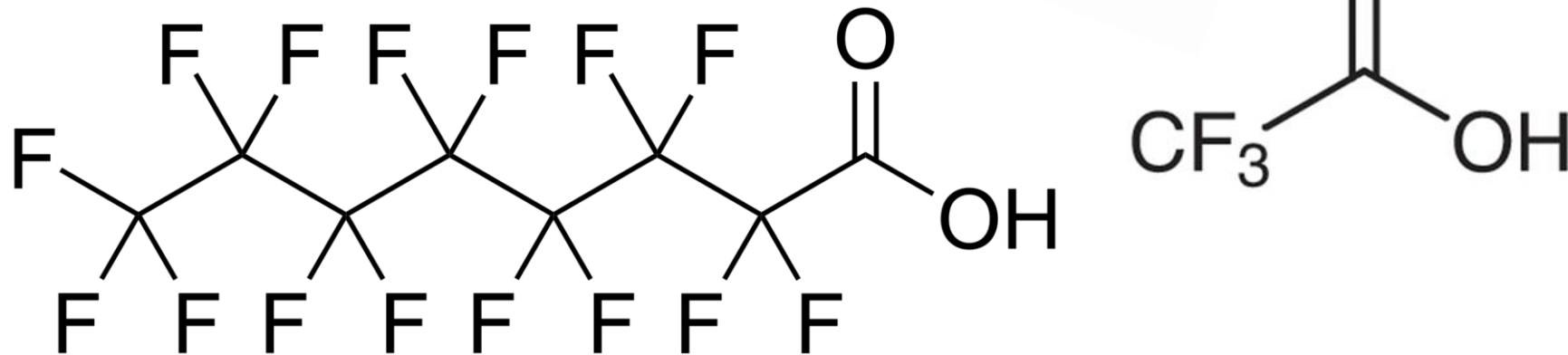
# Charge matters



But...

Activated carbon often struggles with non-aromatic compounds such as

- **1,4-Dioxane**
- **Trifluoroacetic acid**
- **PFAS**



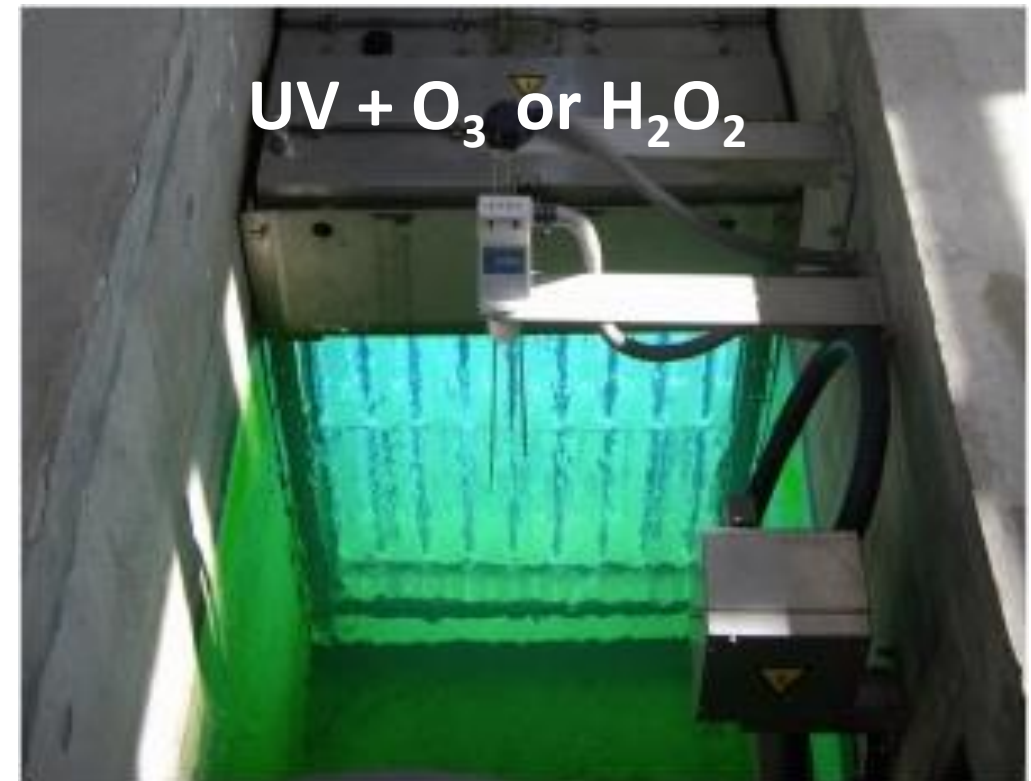
# What is the alternative?

## Reverse Osmosis



[progressivewater.com](http://progressivewater.com)

## Advanced oxidation processes



[ecotechnologies.co.nz](http://ecotechnologies.co.nz)

# What is the alternative?

## Reverse Osmosis



**avoid emissions in the first place**

[progressivewater.com](http://progressivewater.com)

## Advanced oxidation processes



**threat point sources**

[ecotechnologies.co.nz](http://ecotechnologies.co.nz)