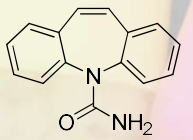
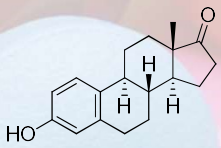
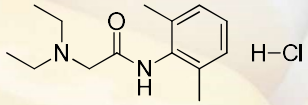
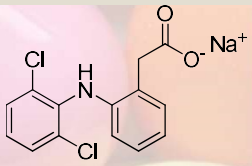
SEDILAB
NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE HUNGARY
PROGRAM FINANCED FROM THE NRDI FUND
MOMENTUM OF INNOVATION
MTA Csillagászati és Földtudományi Kutatóközpont
FÖLDRAJZTUDOMÁNYI INTÉZET

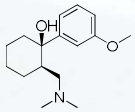


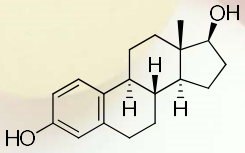


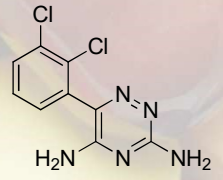


The effect of the chemical properties of EDCs on their adsorption processes to environmental surfaces



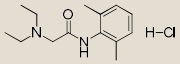


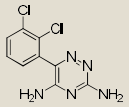


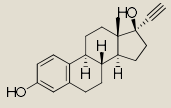


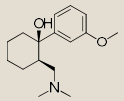
Lili Szabó, Zoltán Szalai , Attila Kondor , Anna Vancsik, Lilla Gáspár, Gergely Jakab, Mariann Ringer and Tibor Filep

Definition of Endocrine-Disrupting Compounds (EDCs)







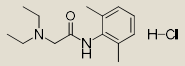


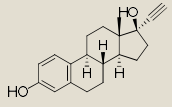
International Programme on Chemical Safety, IPCS

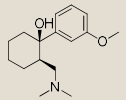
Endocrine disruptors are chemicals that may interfere with the body's endocrine system and produce adverse developmental, reproductive, neurological, and immune effects in both humans and wildlife.

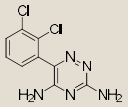
- Pesticides (DDT), dioxin and dioxin-like compounds, Polychlorinated Biphenyl (PCB), plasticizers (bisphenol A)
- Pharmaceuticals (analgesics, birth control pills)
- Heavy metals (Cd, Pb, Hg)

EDCs in the environment









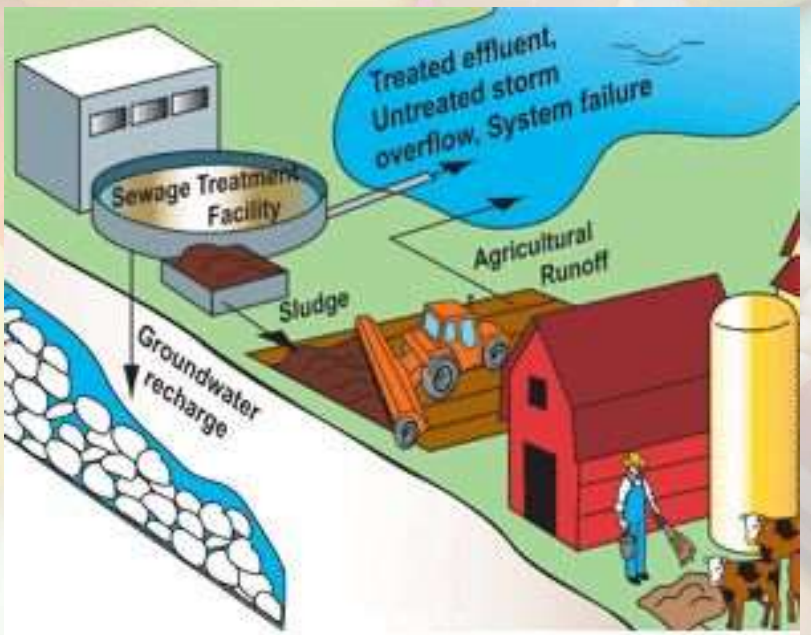
Human and animal medication

Industrial activity (pharmaceutical factories)

Waste water

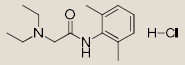
Adsorbed on the wastewater sludge (used in agriculture)

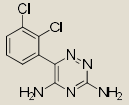
Remained unchanged in the recycled water

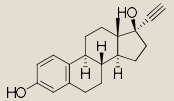


This drawing shows some of the contributions of sewage, biosolids and farms to PPCPs in the environment. (http://www.epa.gov/ppcp/basic2.html)

Objectives







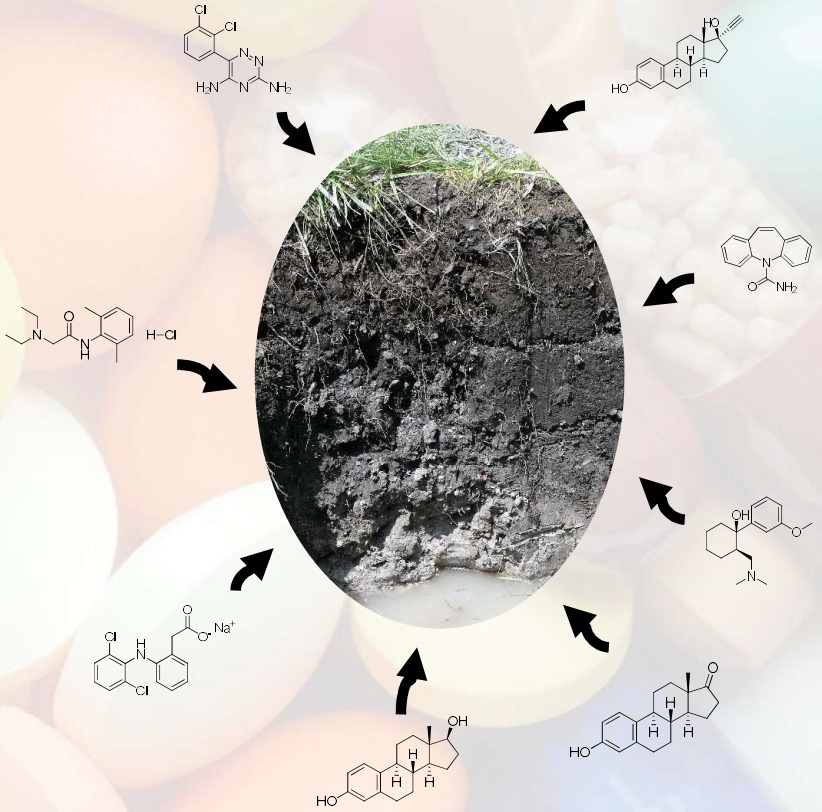
Main objective

The evaluation of the fate and the mobility of EDCs in the environment to assess the risk of the contamination of water, soil and sediments.

- To investigate the effect of octanol-water partition coefficient ($logK_{ow}$) of the drugs on adsorption processes

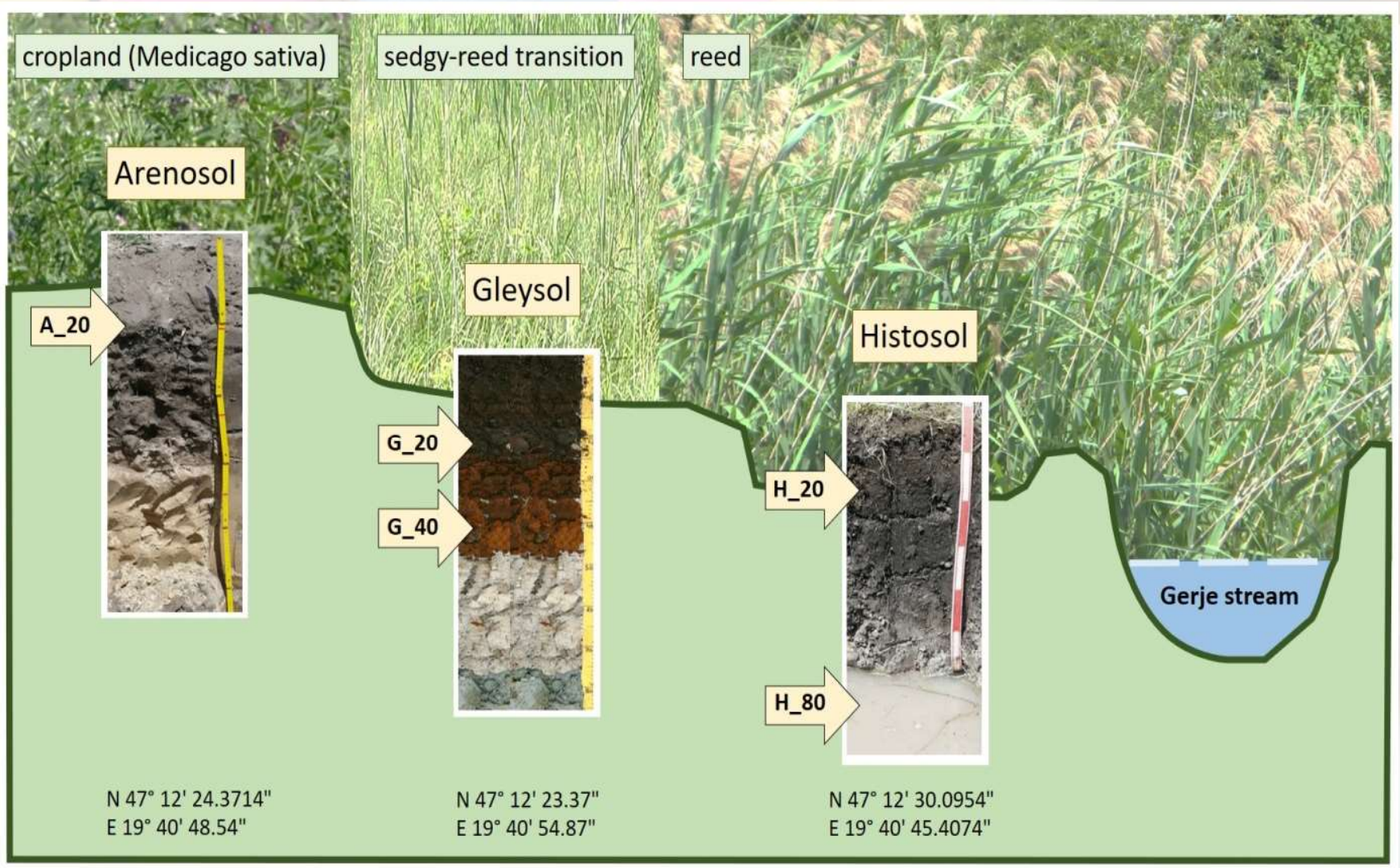
- To assess the relationships between the isotherm parameters and $logK_{ow}$

- To estimate the relations between distribution coefficents (K_D) and $logK_{ow}$

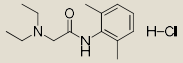


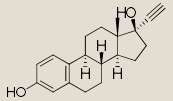
Soil samples

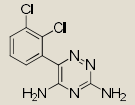
- 3 samples (<250 µm)
- Goethite std.



Physico-chemical properties of the soil samples

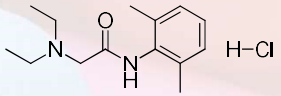


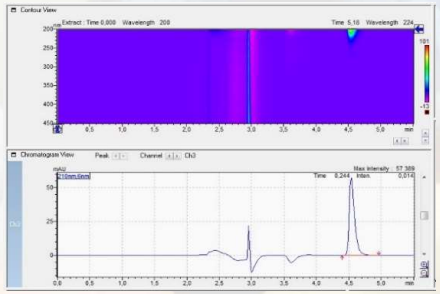


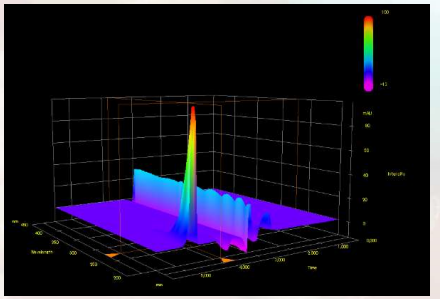


Sorbents	pH (H_2O)	SOC (m/m%)	$CaCO_3$ (m/m%)	Fe (m/m %)	SSA (m^2/g)
Gleysol 20cm	7.3	14.6	36.0	3.0	12.4
Arenosol 20cm	7.9	1.8	11.3	0.9	4.9
Histosol 20cm	7.5	24.4	55.4	1.2	5.6
Goethite std.	3.6	-	-	30-63	11.14

HPLC parameters





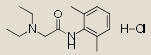


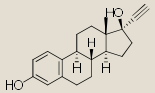
	Total flow (ml/min)	Water/ Acetonitrile (%)	Column temperature (°C)	Ret.time (min)	UV λ (nm)	Fluorescence λ (nm)
EE2	0.5	50/50	40	7.2	-	Ex: 280 Em: 310
E2	0.7	50/50	40	4.6	-	Ex: 280 Em: 310
E1	0,7	50/50	40	6.1	-	Ex: 280 Em: 310
Tramadol	0.8	28/72	22	6.1	-	Ex: 280 Em: 310
Lidocaine	0.6	80/20	30	4.5	210	-
Lamotrigine	0.9	77/23	40	3.2	230	-
Carbamazepine	1	50/50	40	6.5	285	-
Diclofenac-Na	1	40/60	40	3.6	276	-

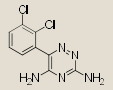
HPLC (Shimadzu Prominance LC-20AR) PDA/FLU

SunShell C18 column

Batch adsorption experiments



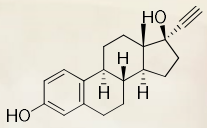
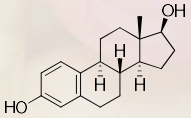
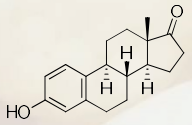
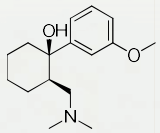
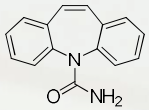
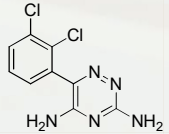
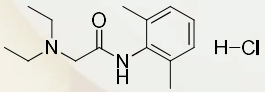
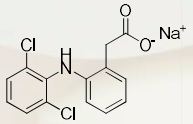


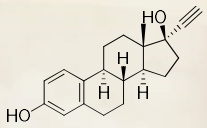
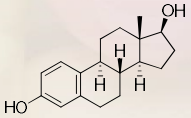
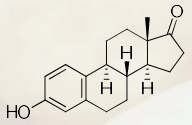
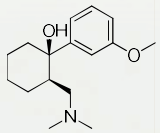
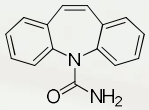
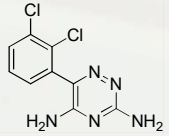
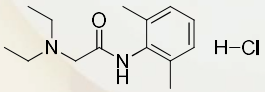
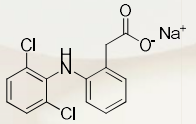


- Soil solution ratio: 1:12
- Rotation: 2 hours (50 rpm)
- Centrifugation: 10 mins (5200 rpm)
- Filtering: glass filter (0.45 µm)

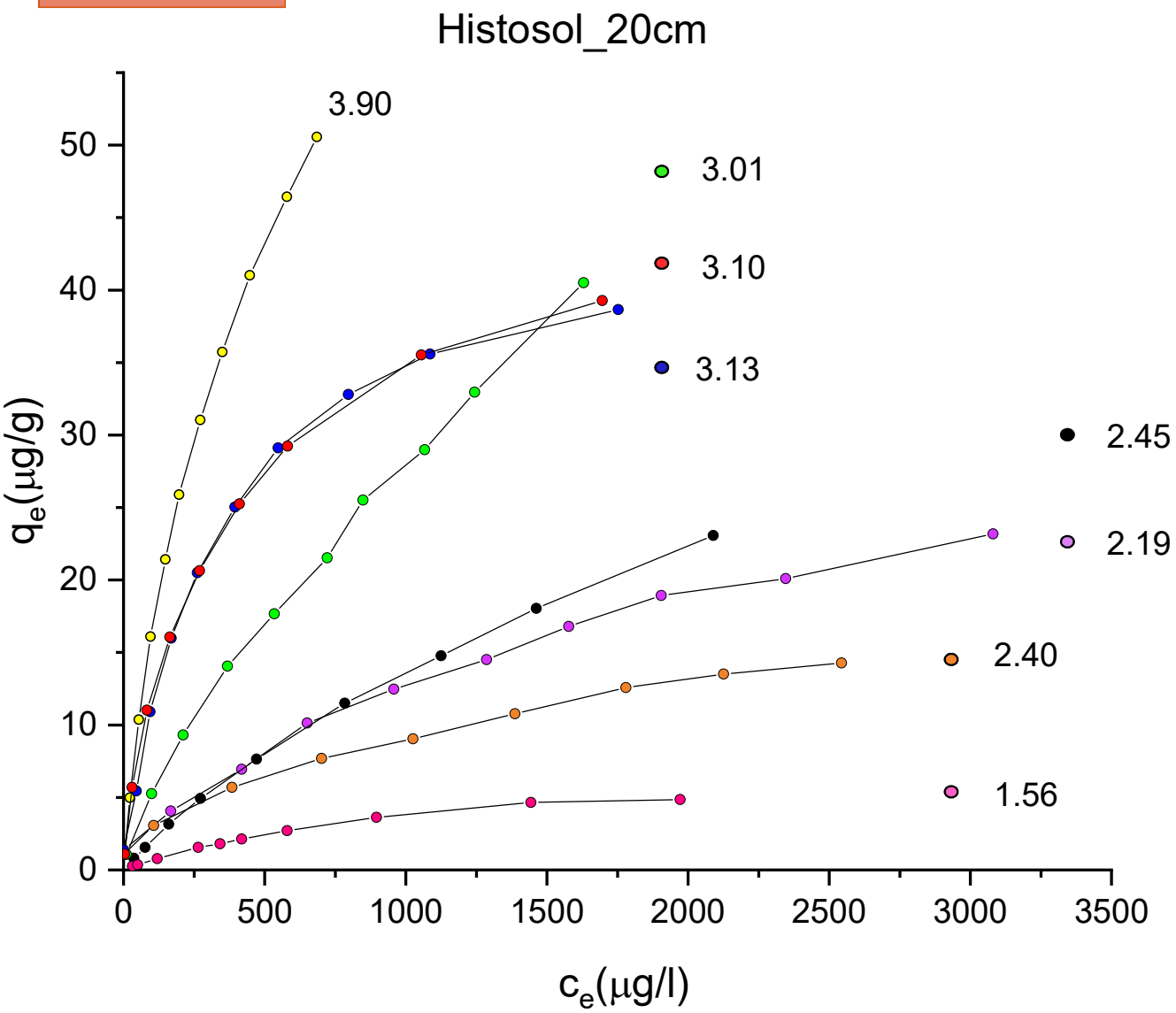
Adsorption models used:

- Langmuir → Q_{max} (µg/g)
- Dubinin-Raduskevich → E (kJ/mol)
- Distribution coefficient → K_D

Pharmaceuticals	n-octanol/water partition coefficient logKow	Dissociation constant pKa_1	Water solubility (mg/l)
EE2 	3.90	10.40	9.20
E2 	3.13	10.34	1.51
E1 	3.10	10.46	1.30
Tramadol-HCl 	3.01	9.41	1151
Carbamazepine 	2.25	14.0	17.66
Lamotrigine 	2.19	8.53	170
Lidocaine-HCl 	2.40	2.19	4100
Diclofenac-Na 	1.56	4.16	5000

Pharmaceuticals	n-octanol/water partition coefficient logKow	Dissociation constant pKa_1	Water solubility (mg/l)
EE2 	3.90	10.40	9.20
E2 	3.13	10.34	1.51
E1 	3.10	10.46	1.30
Tramadol-HCl 	3.01	9.41	1151
Carbamazepine 	2.25	14.0	17.66
Lamotrigine 	2.19	8.53	170
Lidocaine-HCl 	2.40	2.19	4100
Diclofenac-Na 	1.56	4.16	5000

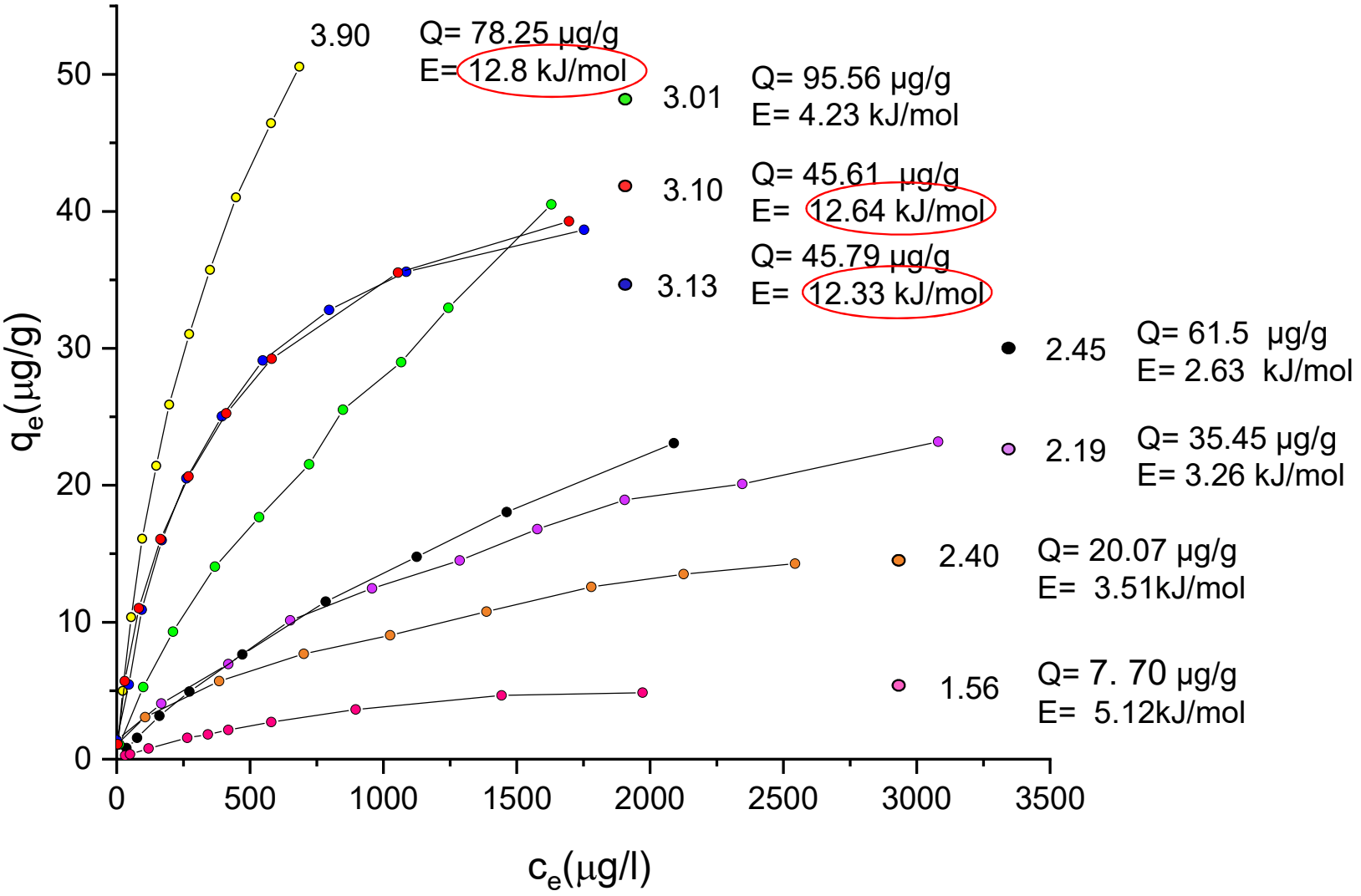
$\log K_{ow}$



- Tramadol
- Lamotrigine
- Carbamazepine
- Diclofenac-Na
- Lidocaine
- EE2
- E2
- E1

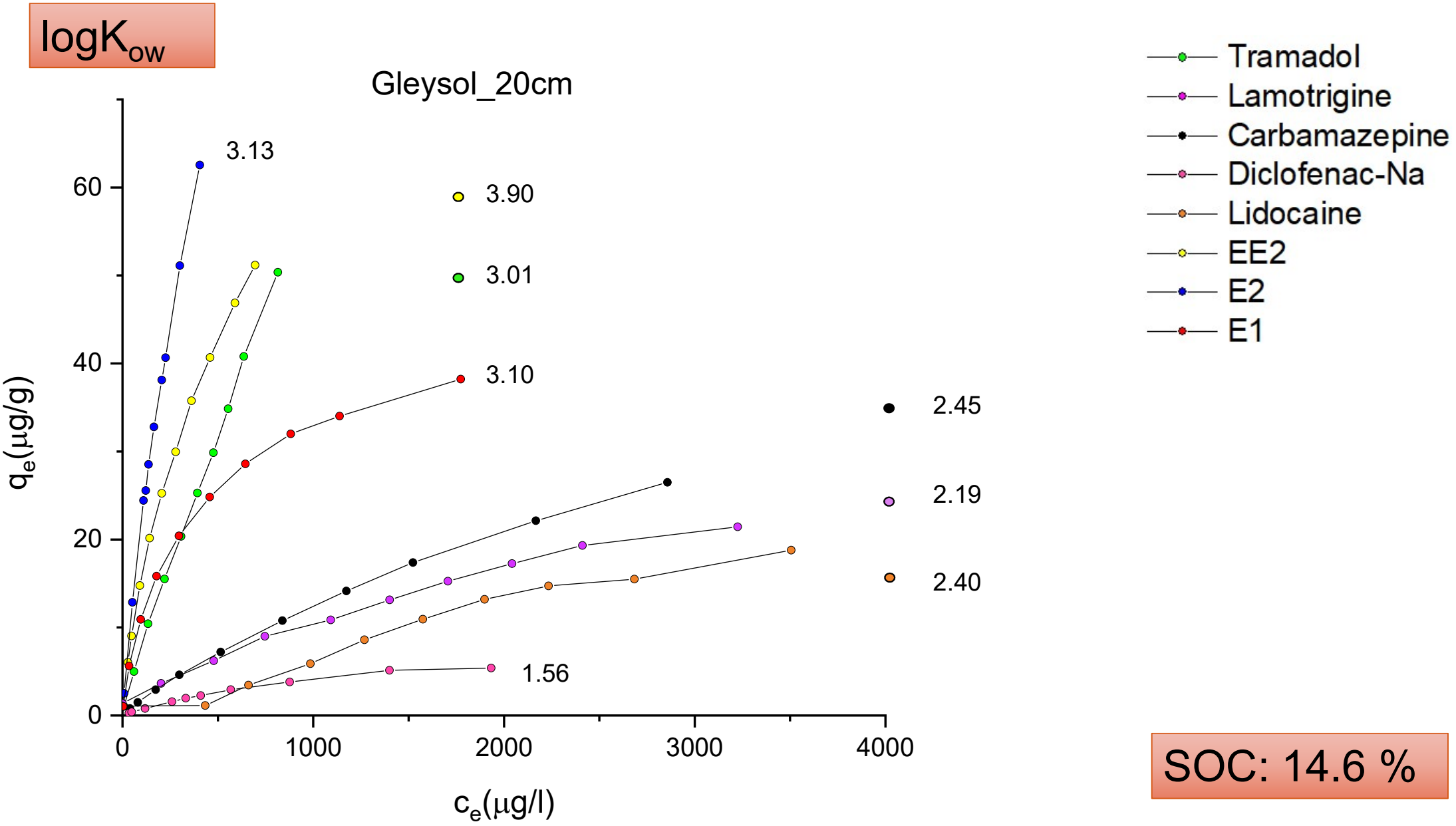
SOC: 24.4 %

$logK_{ow}$, Q_{max}, E

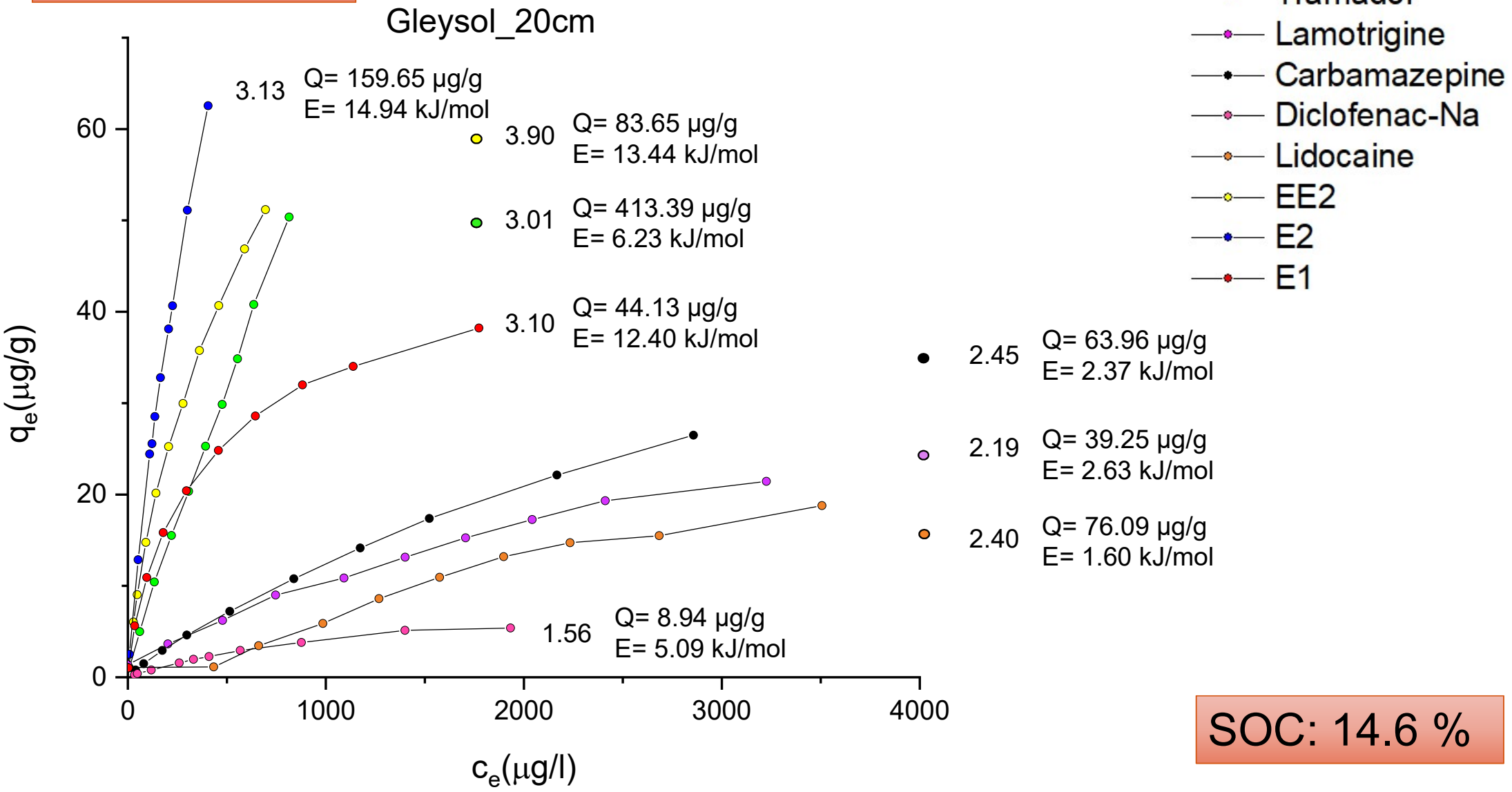


- Tramadol
- Lamotrigine
- Carbamazepine
- Diclofenac-Na
- Lidocaine
- EE2
- E2
- E1

SOC: 24.4 %

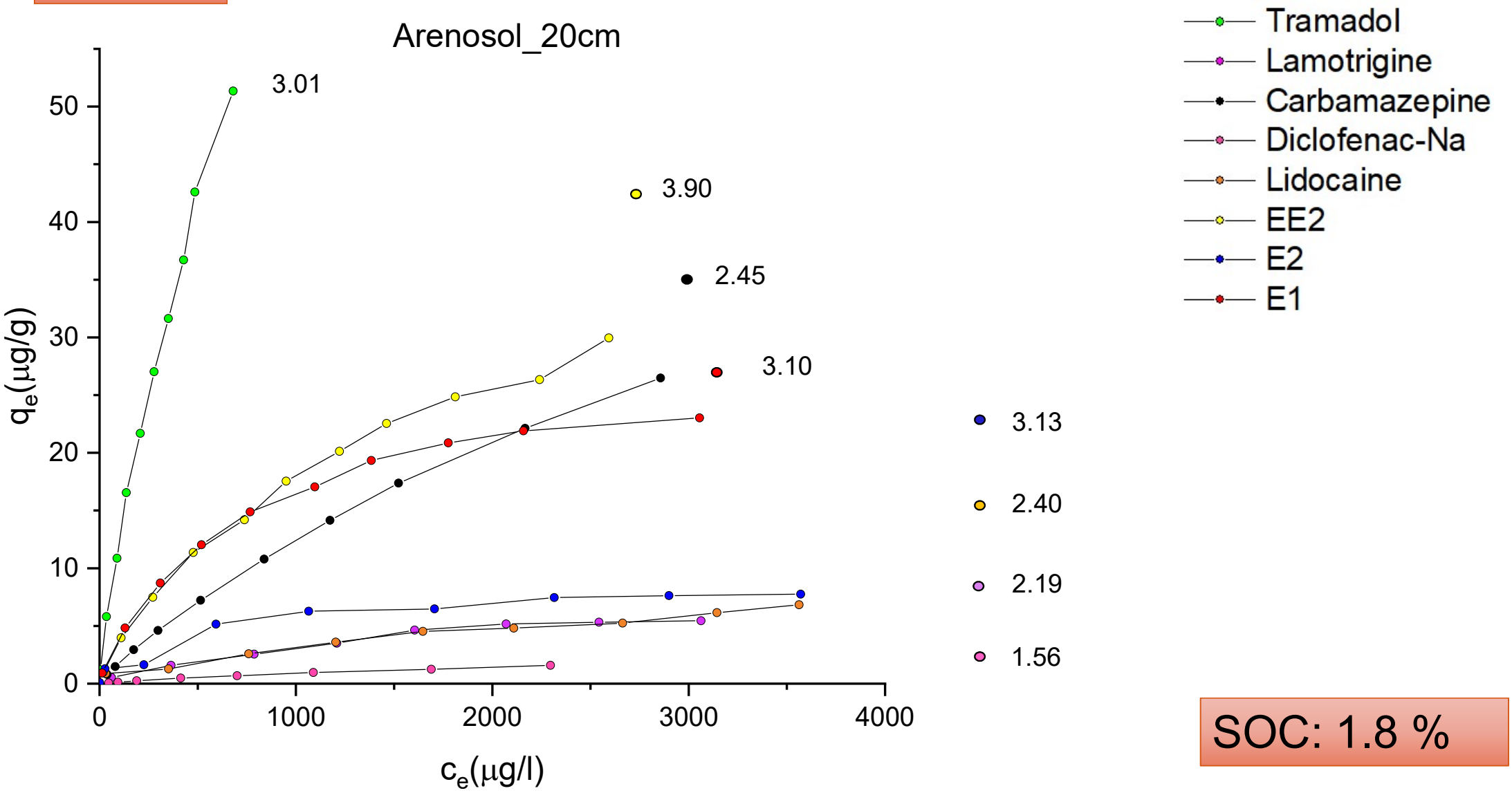

logK$_{ow}$
Gleysol_20cm
3.13
3.90
3.01
3.10
2.45
2.19
2.40
1.56
60
40
20
0
0
1000
2000
3000
4000
q_e(µg/g)
c_e(µg/l)
Tramadol
Lamotrigine
Carbamazepine
Diclofenac-Na
Lidocaine
EE2
E2
E1
SOC: 14.6 %

$\log K_{ow}$, Q_{max}, E



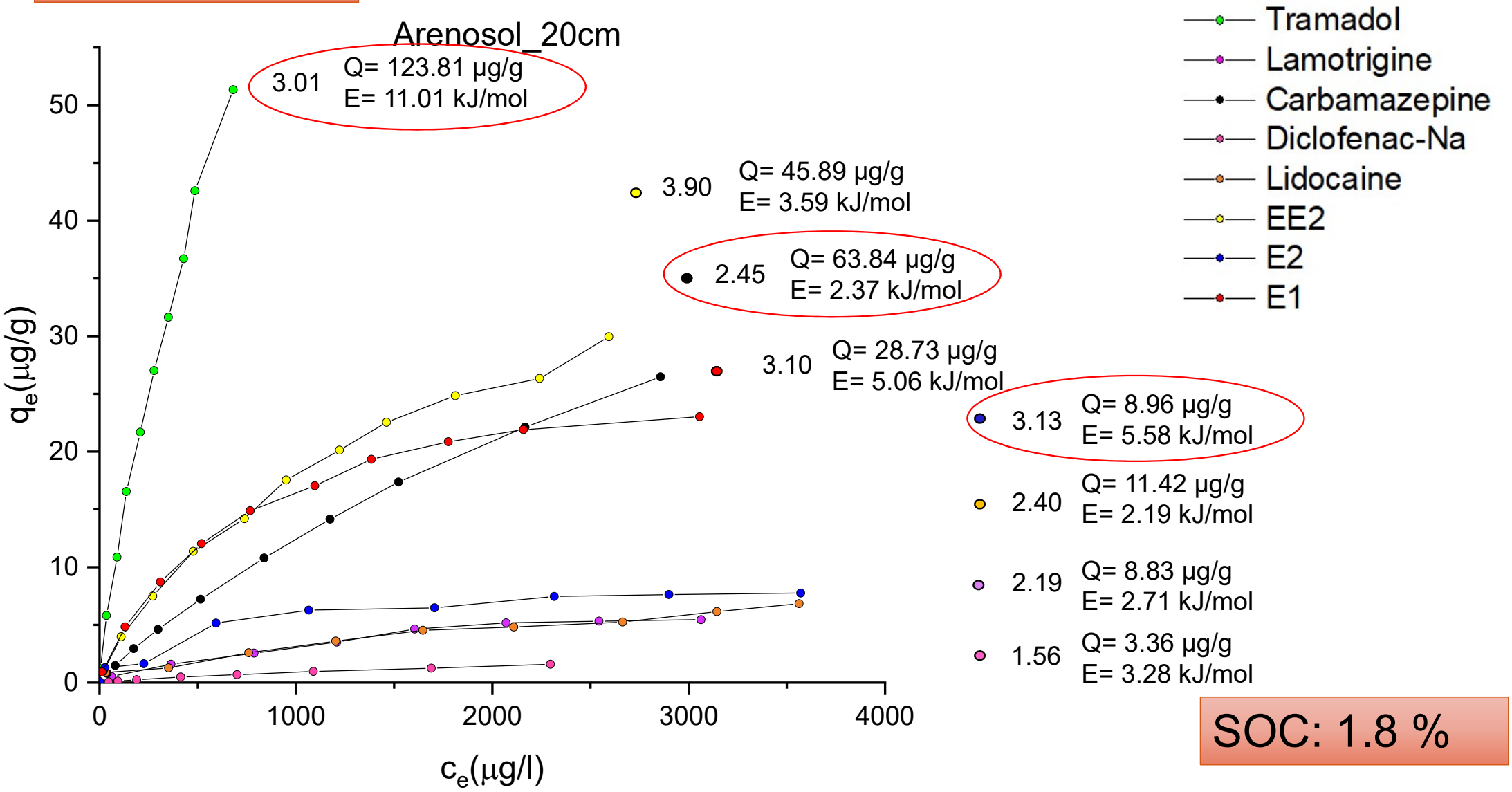
SOC: 14.6 %

$\log K_{ow}$



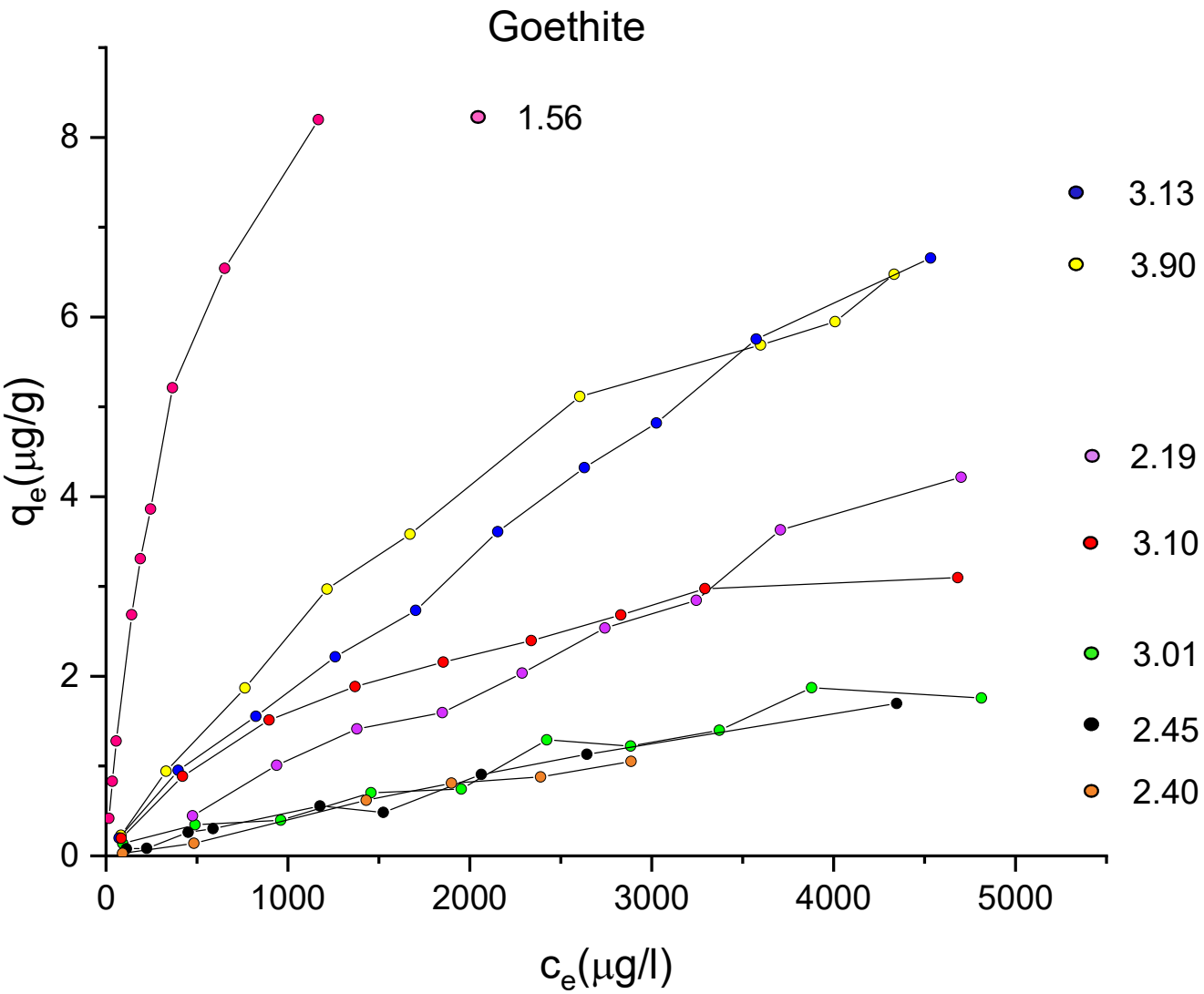
SOC: 1.8 %

$\log K_{ow}$, Q_{max}, E



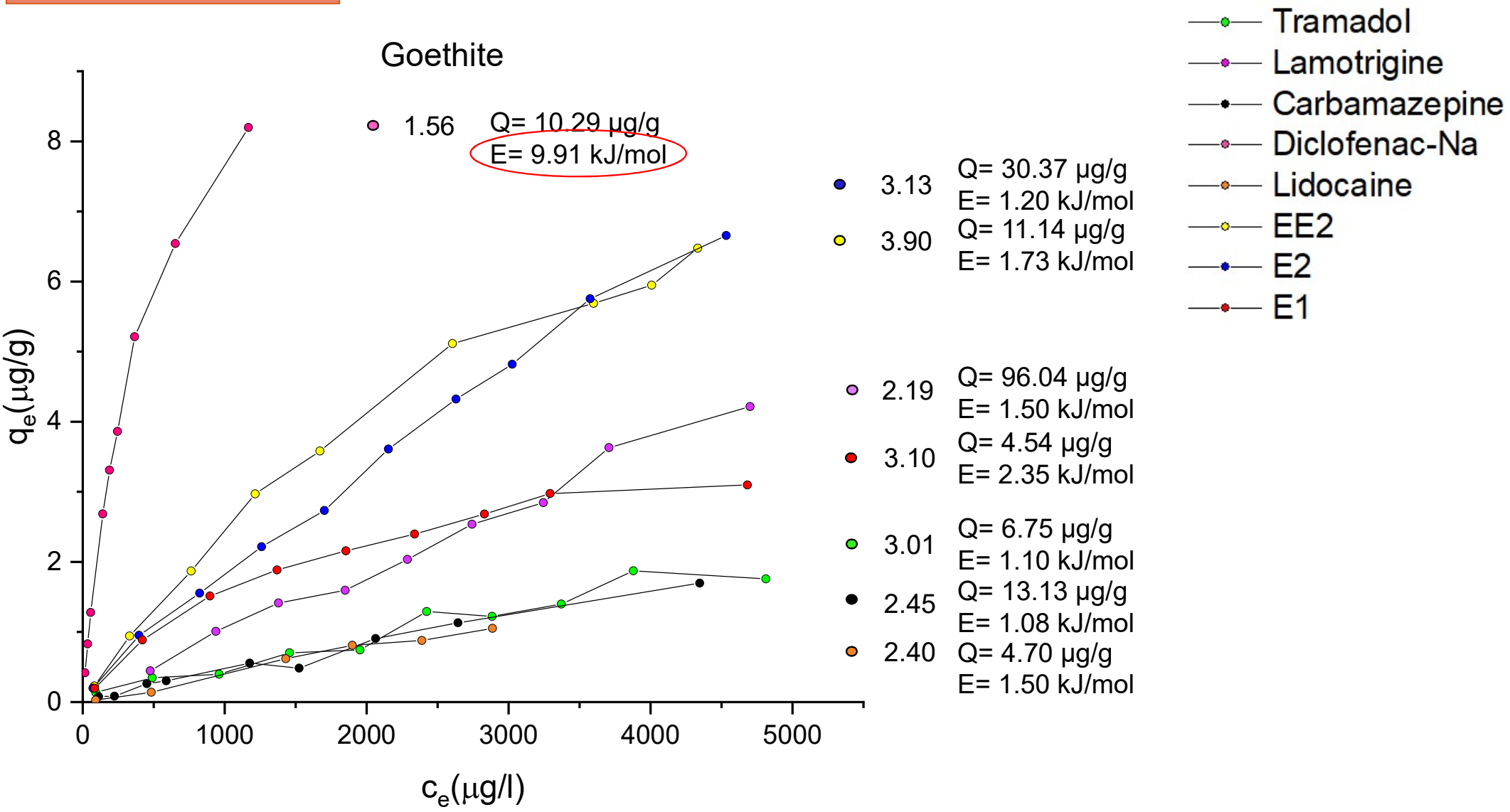
SOC: 1.8 %

$\log K_{ow}$

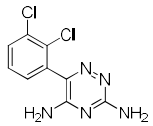


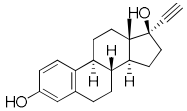
Tramadol
Lamotrigine
Carbamazepine
Diclofenac-Na
Lidocaine
EE2
E2
E1

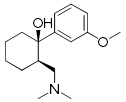
$\log K_{ow}$, Q_{max}, E

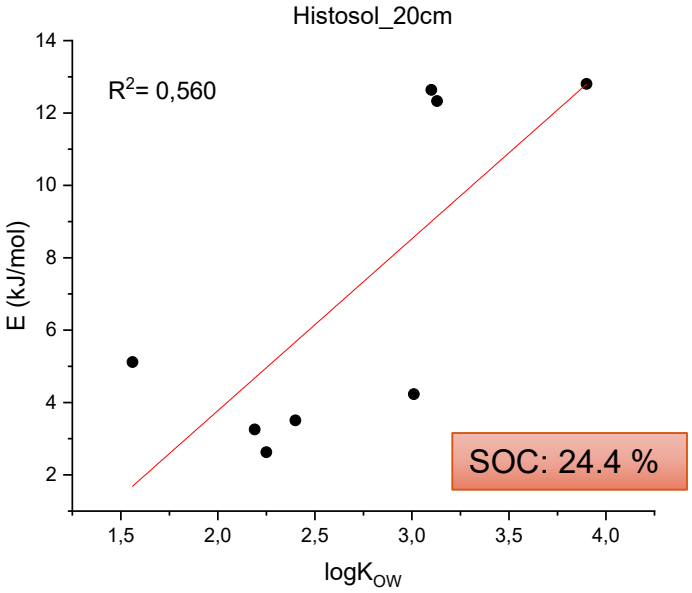


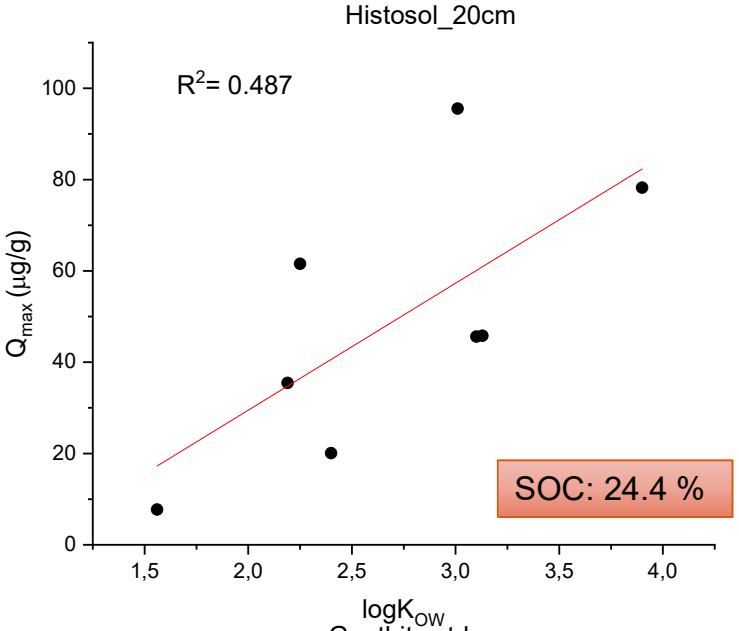
Relationship between $logK_{OW}$ and E, Q_{max}

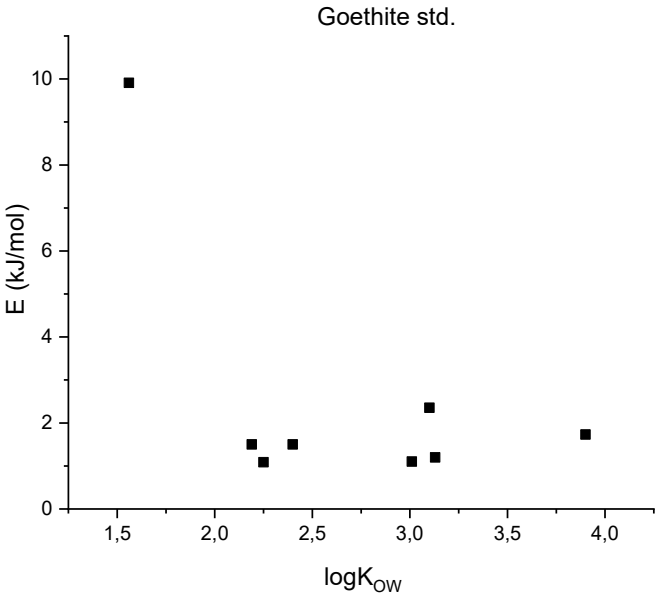


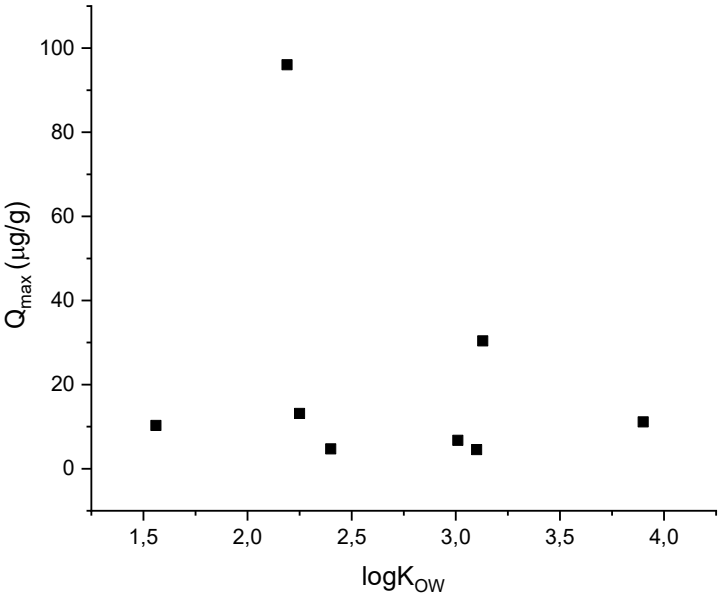






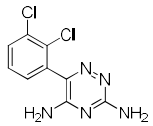


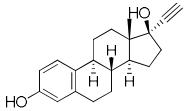


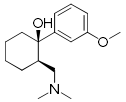


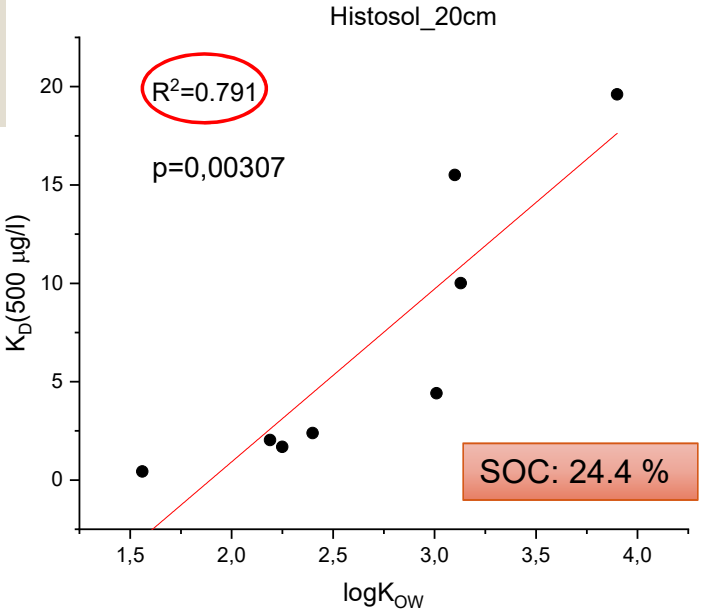
SEDILAB
NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE HUNGARY
PROGRAM FINANCED FROM THE NRDI FUND
MOMENTUM OF INNOVATION

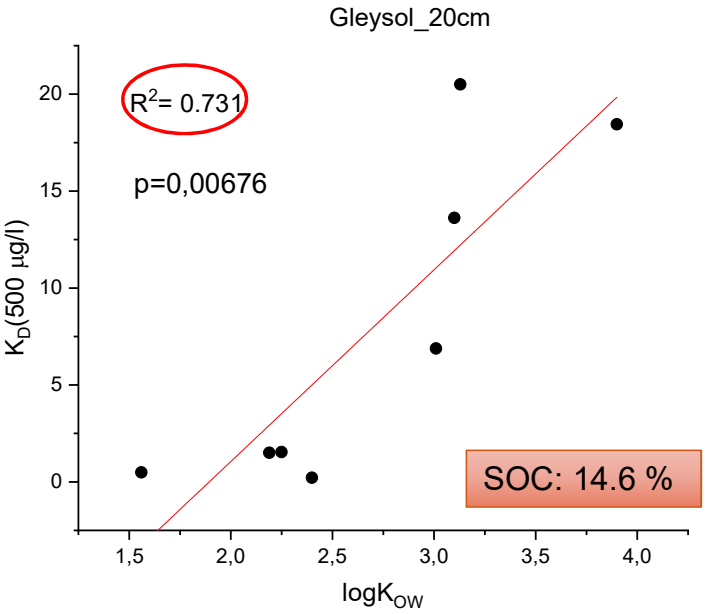
Relationship between $logK_{OW}$ and K_D

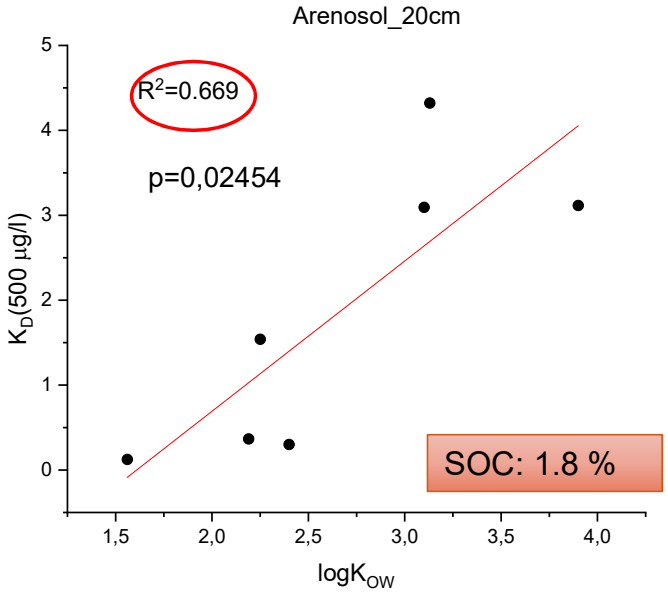


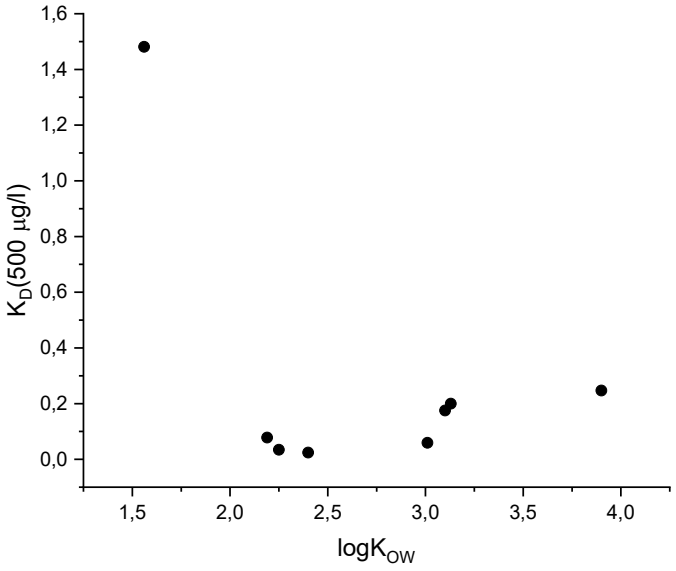






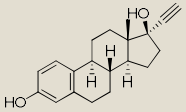


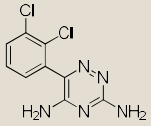


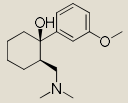


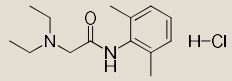
SEDILAB
NATIONAL RESEARCH, DEVELOPMENT AND INNOVATION OFFICE HUNGARY
PROGRAM FINANCED FROM THE NRDI FUND
MOMENTUM OF INNOVATION

Summary









PROGRAM FINANCED FROM THE NRDI FUND
MOMENTUM OF INNOVATION

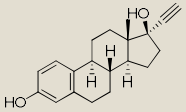
1. The chemical properties of the drugs characterized by $\log K_{ow}$ have great influence on the adsorption of the molecules

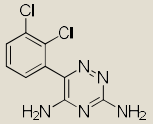
2. Strong relations were found between $Q_{max,}$ E and $\log K_{ow}$ for the soil samples with high organic matter content

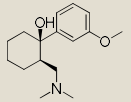
3. Strength of the relationships became weaker with decreasing of organic matter content

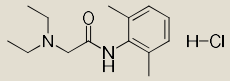
4. There were strong relationships between the K_D and $\log K_{ow}$ values for all soils, however, in the case of goethite there was no correlation

Conclusions





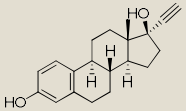


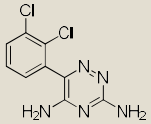


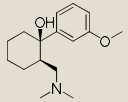
SOM

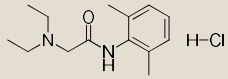
- The $logK_{OW}$ was found to be a good indicator for assessing the adsorption of pharmaceuticals in soils with high organic matter content.
- The ability of the $logK_{ow}$ to evaluate the sorption processes in the soil is limited when the organic matter content is low.
- For mineral compounds, such as goethite, the $logK_{ow}$ of the drugs was found insufficient to describe the sorption.

THANK YOU FOR YOUR ATTENTION!









This study was funded by the Hungarian National Research, Development and Innovation Fund (NVKP_16-1-2016-0003).

SEDILAB

MTA CSFK Laboratory for Sediment and Soil Analyses