Electronic Supplementary Information for "Kaolinite Sorption Isotherms of Benzalkonium and Dialkyldimethylammonium Compounds under Dilute Conditions Investigated by Direct and Passive Sampling Methods"

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S-1. LC/MSD conditions

Instrument: Agilent single quad. LC/MSD
Column: Kinetex 2.6 µm EVO C18 100A, 5.0 x 2.1 mm
Flow rate: 0.25 mL/min
Oven temp.: 40 °C
Detector polarity: Positive
Drying gas flow: 11 L/min (C6, C8, C10-BACs), 10 L/min (C12, C14-BACs, C8-C8-, C10-C10-DADMACs)
Drying gas temp.: 350 °C
Fragmentor voltage: 70 V
Injection volume: 2 µL

Gradient conditions:
Eluent A, water w/ 10 mM NH_4CH_3COO; B, isopropanol w/ 0.1%(v/v) HCOOH; C, acetonitrile

C6, C8, C10-BACs			
Time (min)	Eluent A (%)	Eluent B (%)	Eluent C (%)
0.00	95	0	5
0.05	95	0	5
1.00	40	0	60
5.50	20	0	80
7.50	20	0	80
7.80	95	0	5
12.00	stop		

C12, C14-BACs			
Time (min)	Eluent A (%)	Eluent B (%)	Eluent C (%)
0.00	95	0	5
1.00	30	0	70
5.50	20	0	80
7.50	20	0	80
7.80	95	0	5
12.00	stop		

C8-C8, C10-C10-DADMACs			
Time (min)	Eluent A (%)	Eluent B (%)	Eluent C (%)
0.00	47	2	51
3.00	47	2	51
3.50	17.5	10	72.5
8.00	17.5	10	72.5
8.50	47	2	51
14.00	stop		

MS acquisitions:

	m/z
C6-BAC	220.0
C8-BAC	248.0
C10-BAC	276.0
C12-BAC	304.0
C14-BAC	332.0
C8-C8-DADMAC	270.3
C10-C10-DADMAC	326.3
D_5-C10-BAC	281.0
D_5-C12-BAC	309.0
D_{25}-C12-C12-DADMAC	407.6

Table S1. Freundlich and Langmuir-Freundlich parameters and sorption coefficients obtained for PA fiber sorption of cationic surfactants (15 mM NaCl, pH 7, 25°C) ***in the absence of kaolinite***.

	C6-BAC	C8-BAC	C10-BAC	C12-BAC	C14-BAC	C8-C8-DADMAC	C10-C10-DADMAC
Log $K_{Fr,PA}$	1.53	2.21	2.98	3.60	3.86	3.09	3.77
$n_{Fr,PA}$	0.85	0.76	0.71	0.38	0.37	0.47	0.26
R^2	0.999	0.988	0.966	0.965	0.971	0.951	0.928
Log $q_{max,PA}$	na[a]	3.36	3.58	4.01	4.26	3.69	4.15
Log $K_{LF,PA}$	na[a]	-1.08	-0.30	-0.05	-0.13	-0.43	-0.11
$n_{LF,PA}$	na[a]	0.95	0.94	0.62	0.52	0.81	0.56
R^2	na[a]	0.999	0.994	0.994	0.987	0.994	0.983

[a] Langmuir-Freundlich parameters cannot uniquely be determined.

Table S2. Freundlich parameters and sorption coefficients obtained for PA fiber sorption of cationic surfactants (15 mM NaCl, pH 7, 25°C) ***in the presence of kaolinite***.

	C6-BAC	C8-BAC	C10-BAC	C12-BAC	C14-BAC	C8-C8-DADMAC	C10-C10-DADMAC
Log $K_{Fr,PA}$	1.73	2.42	3.03	3.63	3.81	3.21	3.84
$n_{Fr,PA}$	0.78	0.73	0.64	0.50	0.37	0.39	0.31
R^2	0.998	0.987	0.978	0.921	0.942	0.972	0.917

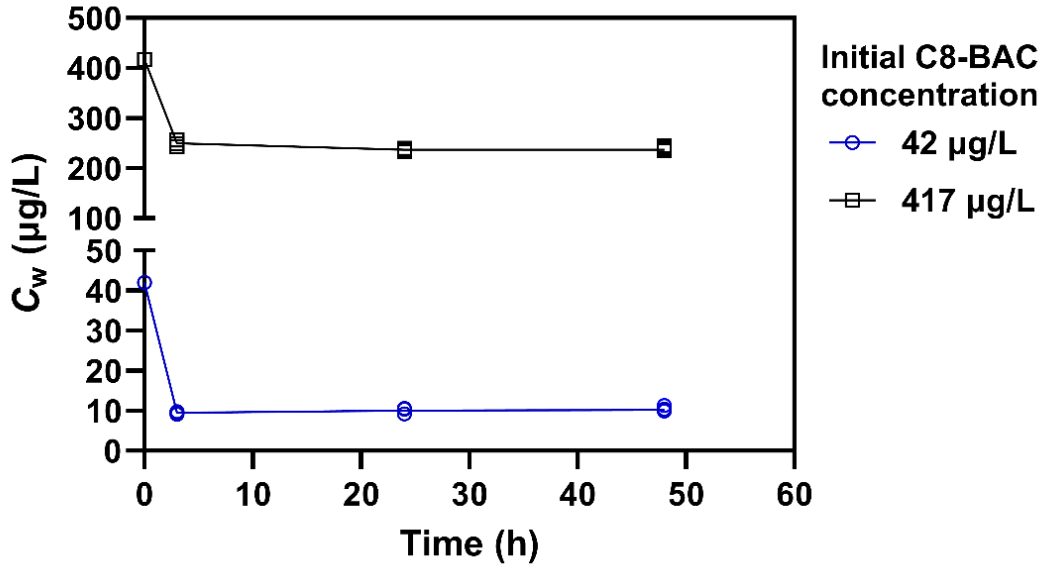

Figure S1. Sorption kinetics of C8-BAC to kaolinite.

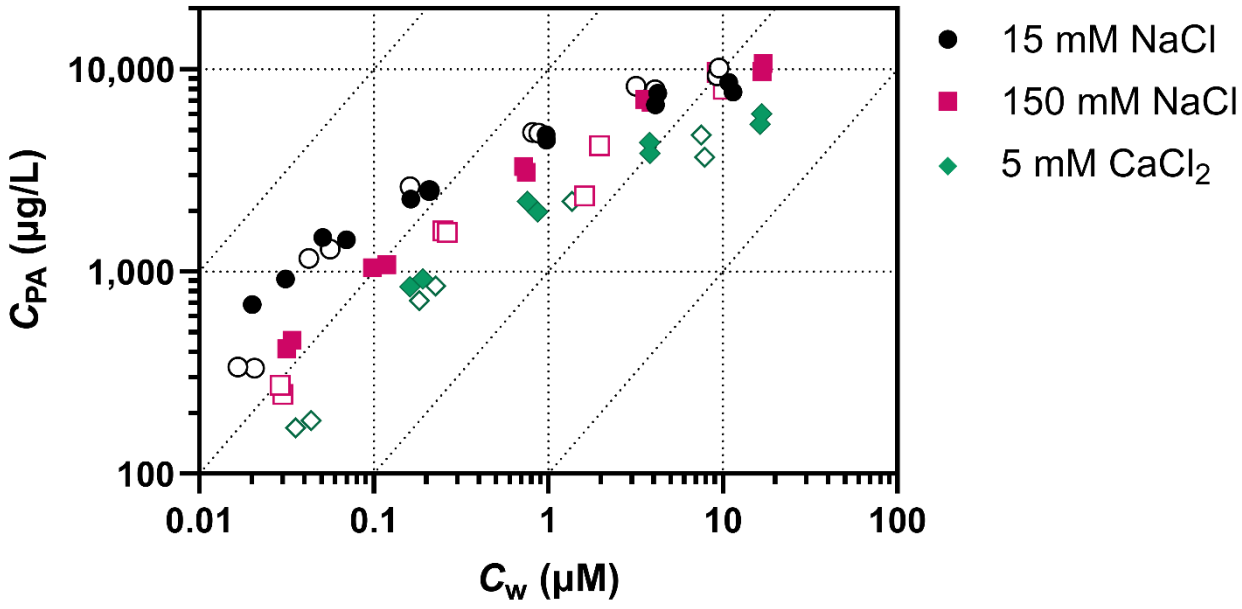

Figure S2. Effect of salt on the PA–water sorption isotherms of C12-BAC. Open and filled symbols indicate the data measured in the presence and absence of kaolinite, respectively.

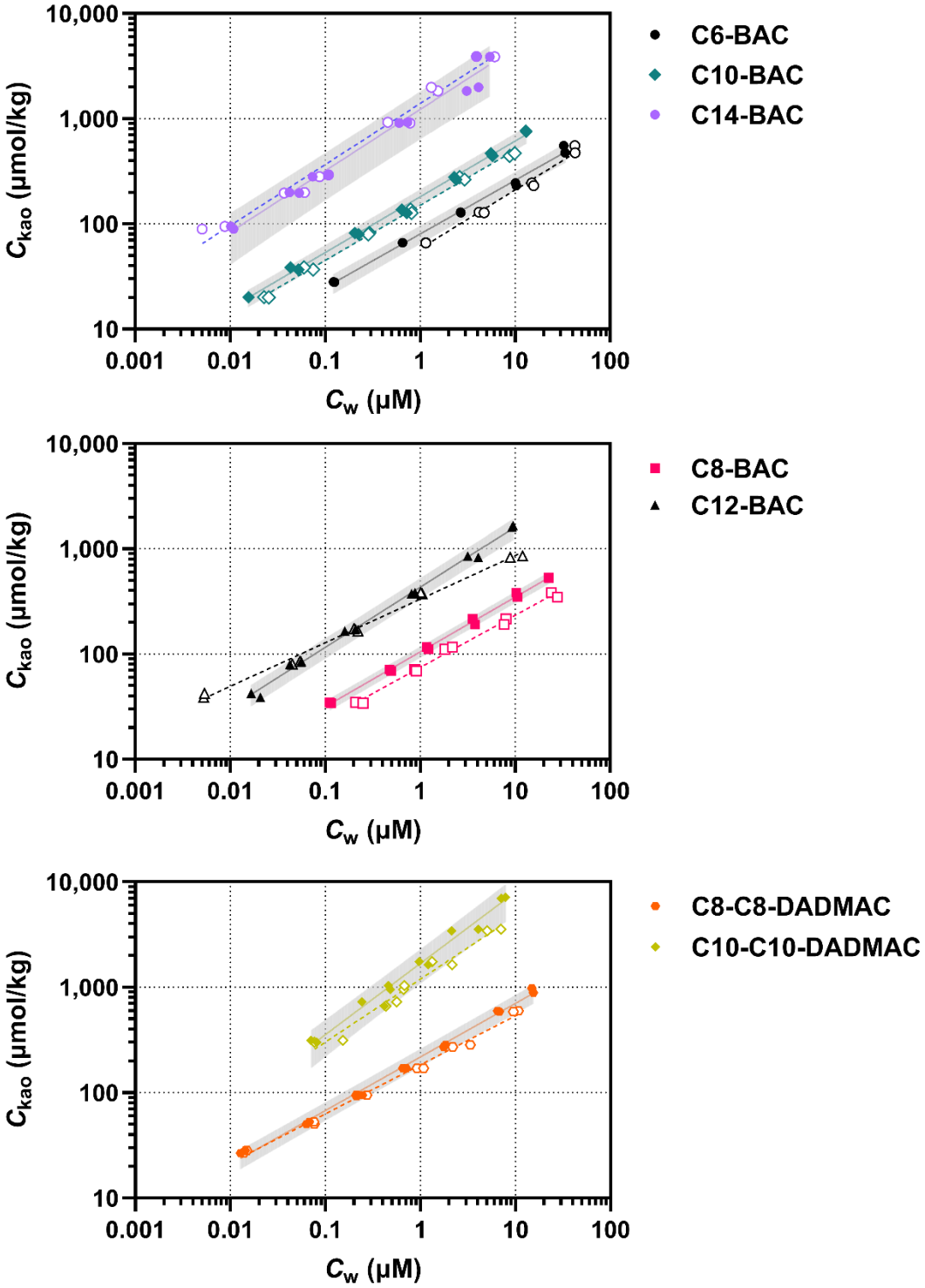

Figure S3. Kaolinite–water sorption isotherms measured by passive and direct sampling methods. Open and filled symbols indicate that C_w was measured by the passive and direct sampling methods, respectively. The lines indicate the fit of the Freundlich equation (eq 3), and the bands indicate the 95% prediction intervals of the fit for the data measured by the direct sampling method.