Table S1:

Supporting Information for the article

"Prediction of critical micelle concentration for per- and polyfluoroalkyl substances"

Benoit Creton[a]*, Eddy Barraud[a], Carlos Nieto-Draghi[a]

[a] IFP Energies nouvelles, 1 et 4 avenue de Bois-Préau, 92852 Rueil-Malmaison, France.

*benoit.creton@ifpen.fr

SMILES	Fold	CMC pred. (mM)	<CMCexp>	Log <CMCexp>	Ref, cf. article
O=C([O-])C(F)(F)C(F)(F)C(F)(F)F.[H+]	0	5.490E+02	7.587E+02	5.880	[30, 31, 20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	3	2.290E+02	1.997E+02	5.300	[30, 31, 20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	5	8.560E+01	8.745E+01	4.942	[30, 31, 20]
O=C([O-])C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[H+]	5	7.775E+01	7.943E+01	4.900	[20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	Val	2.934E+01	2.556E+01	4.408	[30, 31, 20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	4	9.475E+00	8.884E+00	3.949	[30, 31, 20, 33]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[H+]	1	1.424E+01	1.026E+01	4.011	[20, 33]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	5	2.967E+00	2.905E+00	3.463	[30,31,,34]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(C(F)(F)F)C(F)(F)F.[H+]	2	5.576E+00	8.511E+00	3.930	[20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	4	9.288E-01	1.041E+00	3.017	[30, 31, 20]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	3	2.993E-01	3.200E-01	2.505	[31]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	2	1.022E-01	1.000E-01	2.000	[31]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	2	5.190E+02	5.080E+02	5.706	[31]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	5	2.102E+02	2.058E+02	5.313	[35]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	Val	7.488E+01	8.424E+01	4.926	[31, 21, , 35]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	3	2.405E+01	3.086E+01	4.489	[31, 21, 33, 23, 24, 35]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[Na+]	Val	3.034E+01	3.100E+01	4.491	[33, 23, 24]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	2	7.181E+00	1.064E+01	4.027	[31, 21, , 35]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Li+]	2	1.103E+01	1.080E+01	4.033	[34, 23, 24]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Mg+]	0	2.735E+00	2.700E+00	3.431	[34]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	4	2.060E+00	9.124E-01	2.960	[35]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[NH4+]	5	2.300E+01	2.350E+01	4.371	[32, 33]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	1	2.685E+01	2.743E+01	4.438	[21, 33, 23, 24]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	1	2.936E+01	3.000E+01	4.477	[33]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F.[Na+]	4	3.025E+01	3.090E+01	4.490	[21]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)F.[NH4+]	1	1.077E+02	1.100E+02	5.041	[21]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[Na+]	5	3.034E+01	3.200E+01	4.505	[21]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[K+]	1	2.936E+01	3.000E+01	4.477	[21]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(C(F)(F)F)C(F)(F)F.[Na+]	2	2.202E+00	2.020E+00	3.305	[21]
O=C([O-])C(F)(OC(F)(F)C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F)C(F)(F)F.[Na+]	Val	6.913E+00	1.286E+01	4.109	[21]
[H+].[O-]CCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0	1.958E+01	2.000E+01	4.301	[30, 32]
O=C([O-])CC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	3	6.488E+01	7.648E+01	4.884	[21]
O=C([O-])CCC(C(F)(F)F)(C(F)(F)F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	4	5.718E+01	2.641E+01	4.422	[21]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	5	2.248E+01	2.200E+01	4.342	[30, 31]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	4	1.013E+01	1.200E+01	4.079	[30, 31]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[H+]	3	3.629E+00	3.552E+00	3.550	[30, 31, 20, 34]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	5	2.248E+01	2.200E+01	4.342	[32, 21]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	Val	4.885E+00	1.000E+01	4.000	[32, 21, 33]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Li+]	3	1.325E+01	6.300E+00	3.799	[33]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	3	4.729E+00	8.000E+00	3.903	[21, 33]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	2	8.498E-01	1.500E+00	3.176	[32, 21]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Na+]	1	1.837E+00	1.700E+00	3.230	[21, 33]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Li+]	4	6.264E+00	6.400E+00	3.806	[34, 23, 24]

O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	1	3.445E-01	3.200E-01	2.505	[21]
NS(=O)(=O)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	0	3.984E-02	3.900E-02	1.591	[30]
C[N+](C)(C)CCCCCCCCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Br-]	5	1.106E+00	1.130E+00	3.053	[21]
C[N+](C)(C)CCCCCCCCCC(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Br-]	1	8.275E-01	8.100E-01	2.908	[21]
C[N+](C)(C)CCCCCCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Br-]	2	3.882E-01	3.800E-01	2.580	[21]
O=C([O-])C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F.[H+]	1	1.370E+02	1.400E+02	5.146	[30]
O=C([O-])C(F)(OC(F)(F)C(F)(F)C(F)(F)F)C(F)(F)F.[NH4+]	3	1.615E+02	1.650E+02	5.217	[30, 31]
O=S(=O)([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)OC(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[K+]	0	1.762E+00	1.800E+00	3.255	[37]
COC=COC=COC=COCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	1	1.958E+00	2.000E+00	3.301	[21]
COC=COC=COC=COCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	4	8.173E-02	8.000E-02	1.903	[21]
COC=COC=COC=COCC(F)(F)C(F)(F)C(F)(F)C(F)(F)F	3	7.831E+00	8.000E+00	3.903	[21]
COC=COC=COC=COCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	2	3.065E-01	3.000E-01	2.477	[21]
OCCOCCOCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	3	2.550E+00	2.500E+00	3.398	[23, 24]
OCCOCCOCCOCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	5	2.861E+00	2.800E+00	3.447	[23, 24]
OCCOCCOCCOCCOCCOCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	1	3.681E+00	3.700E+00	3.568	[23, 24]
OCCOCCOCCOCCOCCOCCOCCOCCSCCC(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F	2	4.698E+00	4.800E+00	3.681	[23, 24]
O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.[Li+]	4	3.230E+01	3.300E+01	4.519	[23, 24]
CCCCCC(=O)[O-].[Na+]	0	1.022E+03	1.000E+03	6.000	[21]
CCCCCCCCCCCCS(=O)(=O)[O-].[Na+]	0	1.267E+01	1.240E+01	4.093	[21, 23, 24]
CCCCCCCCCCS(=O)(=O)[O-].[Na+]	0	3.607E+01	4.285E+01	4.632	[21, 23, 24]
CCCCCCCCCCOCCS(=O)(=O)[O-].[Na+]	0	2.505E+01	1.590E+01	4.201	[21, 23, 24]
CCCCCCCOS(=O)(=O)[O-].[Na+]	0	3.370E+02	4.027E+02	5.605	[21]
CCCCCCCCOS(=O)(=O)[O-].[Na+]	0	1.660E+02	1.268E+02	5.103	[21]
CCCCCCCCCOS(=O)(=O)[O-].[Na+]	0	7.836E+01	8.005E+01	4.903	[21]
CCCCCCCCCCCOS(=O)(=O)[O-].[Na+]	0	1.608E+01	1.264E+01	4.102	[21]
CCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]	0	7.165E+00	7.320E+00	3.865	[21, 23, 24]
CCCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]	0	3.212E+00	1.510E+00	3.179	[21]
CCCCCCCCCCCCCCOS(=O)(=O)[O-].[Na+]	0	1.467E+00	1.890E+00	3.276	[21, 23, 24]
CCCCCCCCCC[N+](C)(C)C.[Br-]	0	5.031E+01	5.900E+01	4.771	[21, 23, 24]
CCCCCCCCCCC[N+](C)(C)C.[Br-]	0	1.370E+01	1.400E+01	4.146	[21, 23, 24]
CCCCCCCCCCCCCC[N+](C)(C)C.[Br-]	0	3.524E+00	3.600E+00	3.556	[21, 23, 24]
CCCCCCCCCCCCCCCC[N+](C)(C)C.[Br-]	0	9.501E-01	9.300E-01	2.968	[21, 23, 24]
CCCCCCCCCCCCCCCCCC[N+](C)(C)C.[Br-]	0	2.960E-01	2.500E-01	2.398	[21]
CCCCCCCCC(O)CO	0	2.350E+00	2.300E+00	3.362	[23, 24]
CCCCCCCCC(O)CCO	0	9.453E-01	2.300E+00	3.362	[23, 24]
CCCCCCCCCCCCC(O)CCO	0	1.328E-02	1.300E-02	1.114	[23, 24]
CCCCCCCCOCCO	0	5.006E+00	4.900E+00	3.690	[23, 24]
CCCCCCCCOCCOCCOCCO	0	6.654E+00	7.500E+00	3.875	[23, 24]
CCCCCCCCOCCOCCOCCOCCOCCO	0	8.928E+00	9.200E+00	3.964	[23, 24]
CCCCCCCCOCCOCCOCCOCCOCCOCCO	0	1.011E+01	9.900E+00	3.996	[23, 24]
CCCCCCCCCCOCCOCCOCCOCCO	0	7.123E-01	6.800E-01	2.833	[23, 24]
CCCCCCCCCCOCCOCCOCCOCCOCCO	0	7.964E-01	7.600E-01	2.881	[23, 24]
CCCCCCCCCCOCCOCCOCCOCCOCCOCCO	0	8.841E-01	9.000E-01	2.954	[23, 24]
CCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	1.022E+00	1.000E+00	3.000	[23, 24]
CCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	3.051E-01	3.000E-01	2.477	[23, 24]
CCCCCCCCCCCCOCCOCCO	0	5.665E-02	3.300E-02	1.519	[23, 24]
CCCCCCCCCCCCOCCOCCOCCO	0	6.013E-02	5.200E-02	1.716	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCO	0	6.538E-02	6.400E-02	1.806	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCOCCO	0	7.210E-02	6.400E-02	1.806	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO	0	8.759E-02	8.200E-02	1.914	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	9.450E-02	1.090E-01	2.037	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCO	0	2.301E-02	4.900E-02	1.690	[23, 24]
CCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO	0	3.096E-02	2.700E-02	1.431	[23, 24]
CCCCCCCCCCCCCOCCOCCOCCOCCOCCO	0	8.777E-03	1.000E-02	1.000	[23, 24]
CCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCO	0	1.093E-02	9.000E-03	0.954	[23, 24]

CCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	4.218E-03	3.500E-03	0.544	[23, 24]
CCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCO	0	1.360E-03	1.660E-03	0.220	[23, 24]
CCCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCO	0	1.569E-03	1.700E-03	0.230	[23, 24]
CCCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	2.055E-03	2.100E-03	0.322	[23, 24]
CCCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	2.715E-03	2.300E-03	0.362	[23, 24]
CCCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	3.034E-03	3.100E-03	0.491	[23, 24]
CCCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	3.984E-03	3.900E-03	0.591	[23, 24]
CCCCCCCCCCC(=O)N(CCO)CCO	0	2.584E-01	2.640E-01	2.422	[23, 24]
CCCCCCNC(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)CO	0	8.124E+01	8.300E+01	4.919	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1	0	3.371E-01	3.300E-01	2.519	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCO)cc1	0	9.539E-02	1.300E-01	2.114	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCO)cc1	0	1.114E-01	9.700E-02	1.987	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCO)cc1	0	1.328E-01	1.300E-01	2.114	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCO)cc1	0	1.602E-01	1.500E-01	2.176	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCOCCO)cc1	0	1.933E-01	2.100E-01	2.322	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCO)cc1	0	2.309E-01	2.500E-01	2.398	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCO)cc1	0	2.703E-01	2.800E-01	2.447	[23, 24]
CC(C)(C)CC(C)(C)c1ccc(OCCOCCOCCOCCOCCOCCOCCOCCOCCO)cc1	0	3.073E-01	3.000E-01	2.477	[23, 24]
CCCCCCCCC=CCCCCCCCC(=O)OC1(OC2(CO)OC(CO)C(O)C2O)OC(CO)C(O)C(O)C1O	0	1.753E-02	5.100E-03	0.708	[23, 24]
CCCCCCCCCC(=O)CC(=O)NC1CCOC1=O	0	6.830E-02	9.700E-02	1.987	[23, 24]
CCCCCC(=O)CC(=O)NC1CCOC1=O	0	2.217E+00	2.170E+00	3.336	[23, 24]
CCCCCCCCCCCC(=O)NC1CCOC1=O	0	6.709E-03	4.000E-03	0.602	[23, 24]
CCCCCCCCCCCCCCCC(=O)NC1CCOC1=O	0	1.635E-04	1.600E-04	-0.796	[23, 24]
CCCCCCCCOCC(O)CO	0	4.570E+00	5.800E+00	3.763	[23, 24]
CCCCCCCCOC1OC(CO)C(O)C(O)C1O	0	1.955E+01	2.500E+01	4.398	[23, 24]
CCCCOCC(O)C(O)C(O)CO	0	6.836E+01	5.800E+01	4.763	[23, 24]
CCCCCCCCCC(=O)OCC(O)C(O)C(O)CO	0	1.537E+00	1.800E+00	3.255	[23, 24]
CCCCCCC(=O)OCC(O)C(O)C(O)CO	0	3.238E+01	1.000E+01	4.000	[23, 24]
CCCCCCCOCC(O)C(O)C(O)CO	0	9.399E+00	9.200E+00	3.964	[23, 24]
CCCCCC(=O)OCC(O)C(O)C(O)CO	0	7.717E+01	5.800E+01	4.763	[23, 24]
CCCCCCOCC(O)C(O)C(O)CO	0	2.220E+01	9.400E+00	3.973	[23, 24]
CCCCCCCCC(=O)OCC(O)C(O)C(O)CO	0	4.495E+00	4.400E+00	3.643	[23, 24]
CCCCCCCCCOCC(O)C(O)C(O)CO	0	1.389E+00	2.100E+00	3.322	[23, 24]
CCCCCCCC(=O)OCC(O)C(O)C(O)CO	0	1.249E+01	1.800E+01	4.255	[23, 24]
CCCCCCCCOCC(O)C(O)C(O)CO	0	3.711E+00	6.700E+00	3.826	[23, 24]
CCCCC(=O)OCC(O)C(O)C(O)CO	0	1.173E+02	1.200E+02	5.079	[23, 24]
CCCCOCC(O)C(O)C(O)CO	0	4.825E+01	3.800E+01	4.580	[23, 24]
CCCCSCC(O)C(O)C(O)CO	0	7.685E+01	1.800E+02	5.255	[23, 24]
CCCCCSCC(O)C(O)C(O)CO	0	4.533E+01	4.600E+01	4.663	[23, 24]
CCCCCC(CCCC)OC1OC(CO)C(O)C(O)C1O	0	1.532E+01	1.500E+01	4.176	[23, 24]
CCCCCCCC(CC)OC1OC(CO)C(O)C(O)C1O	0	1.111E+01	8.500E+00	3.929	[23, 24]
CCCCCCCCC(C)OC1OC(CO)C(O)C(O)C1O	0	4.405E+00	4.500E+00	3.653	[23, 24]
CCCCCCC(CCC)OC1OC(CO)C(O)C(O)C1O	0	9.839E+00	1.200E+01	4.079	[23, 24]
CCCCCCCCCCCC(=O)OCC1OC(OC2C(CO)OC(O)C(O)C2O)C(O)C(O)C1O	0	4.867E-01	3.300E-01	2.519	[23, 24]
CCCCCCCC(CCCCCC)SCCC(=O)OCC1(O)C(O)C(O)C(O)C1O	0	6.436E-03	6.300E-03	0.799	[23, 24]
CCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	0	5.828E+00	6.700E+00	3.826	[23, 24]
CCCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	0	2.002E+01	2.100E+01	4.322	[23, 24]
CCCCCCCC(=O)N(C)CC(O)C(O)C(O)C(O)CO	0	6.754E+01	6.900E+01	4.839	[23, 24]
CCCCCCCCCCCC(=O)OCC1OC(OCC2OC(OC3(CO)OC(CO)C(O)C3O)C(O)C(O)C2O)C(O)C(O)C1O	0	8.676E-01	9.500E-01	2.978	[23, 24]
CCCCCCCCCCCC(=O)OCC1OC(OCC2OC(OCC3OC(OC4(CO)OC(CO)C(O)C4O)C(O)C(O)C3O)C(O)C(O)C2O)C(O)C(O)C1O	0	2.350E+00	2.300E+00	3.362	[23, 24]
CCCCCCCCCCCC(=O)OCC1OC(OC2(CO)OC(CO)C(O)C2O)C(O)C(O)C1O	0	4.503E-01	4.600E-01	2.663	[23, 24]
CCCCCCCCCCSCC(O)C(O)C(O)CO	0	2.337E-01	4.000E-01	2.602	[23, 24]
CCCCCCCCCCSC1OC(=O)C(O)C1O	0	3.440E-02	3.300E-02	1.519	[23, 24]
CCCCCCSCC(O)C(O)C(O)CO	0	1.700E+01	1.200E+01	4.079	[23, 24]
CCCCCCSC1OC(=O)C(O)C1O	0	6.558E+00	6.700E+00	3.826	[23, 24]

CCCCCCCCSCC(O)C(O)C(O)CO	0	2.076E+00	1.200E+00	3.079	[23, 24]
CCCCCCCCSC1OC(=O)C(O)C1O	0	4.904E-01	4.800E-01	2.681	[23, 24]
CCCCCCCC(=O)NC1C(O)OC(CO)C(O)C1O	0	4.597E+01	4.500E+01	4.653	[23, 24]
CCCCCCCC(=O)NC1OC(CO)C(O)C(O)C1O	0	6.852E+01	7.000E+01	4.845	[23, 24]
CC(C)CCCC(C)CCOC1OC(CO)C(O)C(O)C1O	0	4.087E+00	4.000E+00	3.602	[23, 24]
CC(C)CCCC(C)CCOC1OC(CO)C(OC2OC(CO)C(O)C(O)C2O)C(O)C1O	0	5.188E+00	5.300E+00	3.724	[23, 24]
CC(C)CCCC(C)CCOC1OC(CO)C(OC2OC(CO)C(OC3OC(CO)C(O)C(O)C3O)C(O)C2O)C(O)C1O	0	5.108E+00	5.000E+00	3.699	[23, 24]
CCCCCCCCCOC1OC(CO)C(O)C(O)C1N	0	7.151E+00	7.000E+00	3.845	[23, 24]
CCCCCCCCOC1OC(CO)C(O)C(O)C1N	0	2.251E+01	2.300E+01	4.362	[23, 24]
CCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(O)C(O)CO	0	1.982E+00	1.300E+00	3.114	[23, 24]
CCCCCCCCCCN(C)C(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	1.448E+00	2.300E+00	3.362	[23, 24]
CCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(O)C(O)CO	0	1.818E-01	1.400E-01	2.146	[23, 24]
CCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	2.038E-01	2.500E-01	2.398	[23, 24]
CCCCCCCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	9.103E-03	9.300E-03	0.968	[23, 24]
CCCCCCCCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	3.371E-03	3.300E-03	0.519	[23, 24]
CCCCCCCCC=CCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(O)CO	0	3.269E-02	3.200E-02	1.505	[23, 24]
CCCCCCCCC=CCCCCCCCCN(C)C(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	5.286E-02	5.400E-02	1.732	[23, 24]
CCCCCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(O)C(O)CO	0	2.100E-02	2.400E-02	1.380	[23, 24]
CCCCCCCCCCCCCCCN(C)C(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	3.645E-02	3.600E-02	1.556	[23, 24]
CCCCCCCCCCCC(=O)N(C)CC(O)CO	0	2.350E-01	2.300E-01	2.362	[23, 24]
CCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(O)CO	0	4.150E-01	3.600E-01	2.556	[23, 24]
CCCCCCCCCCOC1OC(CO)C(O)C(O)C1O	0	2.037E+00	2.000E+00	3.301	[23, 24]
CCCCCCCCCCOC1OC(CO)C(OC2OC(CO)C(O)C(O)C2O)C(O)C1O	0	2.043E+00	2.000E+00	3.301	[23, 24]
CCCCCCCCCCCOC1OC(CO)C(O)C(O)C1O	0	1.941E-01	1.900E-01	2.279	[23, 24]
CCCCCCCCC=CCCCCCCCC(=O)NCCOC1OC(CO)C(OC2OC(CO)C(O)C(O)C2O)C(O)C1O	0	8.809E-02	9.000E-02	1.954	[23, 24]
CCCCCCCCC=CCCCCCCCCOC1OC(CO)C(OC2OC(CO)C(O)C(O)C(O)C2O)C(O)C1O	0	1.958E-02	2.000E-02	1.301	[23, 24]
CCCCCCCCC=CCCCCCCCCOC1OC(CO)C(OC2OC(CO)C(OC3OC(CO)C(O)C(O)C3O)C(O)C2O)C(O)C1O	0	4.291E-02	4.200E-02	1.623	[23, 24]
CCCCCCCCCCNC(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)CO	0	1.351E+00	1.300E+00	3.114	[23, 24]
CCCCCCCCCCCCNC(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)CO	0	1.935E-01	3.100E-01	2.491	[23, 24]
CCCCCCCCCCCCOC1OC(CO)C(OC2OC(CO)C(O)C(O)C2O)C(O)C1O	0	2.482E-01	1.700E-01	2.230	[23, 24]
CCCCCCCCNC(=O)C(O)C(O)C(OC1OC(CO)C(O)C(O)C1O)C(O)CO	0	1.058E+01	5.700E+00	3.756	[23, 24]
CCCCCCCCCC(=O)N(C)CC(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	3.473E+00	3.300E+00	3.519	[23, 24]
CCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	4.597E-01	4.500E-01	2.653	[23, 24]
CCCCCCCCCCCCCC(=O)N(C)CC(O)C(O)C(OC1OC(CO)C(O)C(O)C(O)C1O)C(O)CO	0	7.347E-02	6.800E-02	1.833	[23, 24]
CCCCCCCCCOC1OC(CO)C(O)C(O)C1O	0	6.449E+00	6.900E+00	3.839	[23, 24]
CCCCCCCCSC1OC(CO)C(O)C(O)C1O	0	8.320E+00	8.500E+00	3.929	[23, 24]
CCCCCCOCCOCCOCCO	0	5.743E+01	1.000E+02	5.000	[23, 24]
CCCCCCCCCCOCCOCCOCCO	0	6.392E-01	6.000E-01	2.778	[23, 24]
CCCCCCCCCCCCOCCOCCOCCOCCOCCOCCO	0	7.977E-02	8.700E-02	1.940	[23, 24]
CCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	1.177E+01	1.300E+01	4.114	[23, 24]
CCCCCCCCCCOCCOCCOCCOCCOCCOCCOCCOCCOCCO	0	1.044E+00	1.300E+00	3.114	[23, 24]
CCCCCCCC[N+](C)(C)C.[Br-]	0	1.576E+02	1.400E+02	5.146	[23, 24]
CCCCCCCCCC[N+](C)(C)C.[Cl-]	0	6.947E+01	6.800E+01	4.833	[23, 24]
CCCCCCCCCCCC[N+](C)(C)C.[Cl-]	0	1.847E+01	2.000E+01	4.301	[23, 24]
CCCCCCCCCCCCCC[N+](C)(C)C.[Cl-]	0	4.597E+00	4.500E+00	3.653	[23, 24]
CCCCCCCCCC[n+]1ccccc1.[Br-]	0	4.495E+01	4.400E+01	4.643	[23, 24]
CCCCCCCCCCC[n+]1ccccc1.[Br-]	0	2.258E+01	2.100E+01	4.322	[23, 24]
CCCCCCCCCCCC[n+]1ccccc1.[Br-]	0	1.109E+01	1.140E+01	4.057	[23, 24]
CCCCCCCCCCCC[n+]1ccccc1.[Cl-]	0	1.664E+01	1.700E+01	4.230	[23, 24]
CCCCCCCCCCCC[n+]1ccccc1.[I-]	0	5.188E+00	5.300E+00	3.724	[23, 24]
CCCCCCCCCCCCC[n+]1ccccc1.[Br-]	0	5.392E+00	5.300E+00	3.724	[23, 24]
CCCCCCCCCCCCCC[n+]1ccccc1.[Br-]	0	2.624E+00	2.700E+00	3.431	[23, 24]
CCCCCCCCCCCCCC[n+]1ccccc1.[Cl-]	0	3.696E+00	3.500E+00	3.544	[23, 24]
CCCCCCCCCCCCCCC[n+]1ccccc1.[Br-]	0	1.294E+00	1.300E+00	3.114	[23, 24]
CCCCCCCCCCCCCCCC[n+]1ccccc1.[Br-]	0	6.538E-01	6.400E-01	2.806	[23, 24]

CCCCCCCCCCCCCCCC[n+]1ccccc1.[Cl-]	0	8.809E-01	9.000E-01	2.954	[23, 24]
CCCCCCCCCCCCCCCCCC[n+]1ccccc1.[Cl-]	0	2.452E-01	2.400E-01	2.380	[23, 24]
CCCCCCCCCCC[N+](C)(C)CC.[Br-]	0	1.364E+01	1.400E+01	4.146	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCC.[Br-]	0	9.195E+00	7.500E+00	3.875	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCCCC.[Br-]	0	3.754E+00	3.100E+00	3.491	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCCCCCC.[Br-]	0	1.124E+00	1.100E+00	3.041	[23, 24]
CCCCCCCCCCCCCC[N+](CC)(CC)CC.[Br-]	0	3.034E+00	3.100E+00	3.491	[23, 24]
CCCCCCCCCCCCCC[N+](CCC)(CCC)CCC.[Br-]	0	2.145E+00	2.100E+00	3.322	[23, 24]
CCCCCCCCCCCCCC[N+](CCCC)(CCCC)CCCC.[Br-]	0	1.226E+00	1.200E+00	3.079	[23, 24]
CCCCCCCCCC[N+](C)(C)Cc1ccccc1.[Cl-]	0	3.817E+01	3.900E+01	4.591	[23, 24]
CCCCCCCCCCCC[N+](C)(C)Cc1ccccc1.[Cl-]	0	8.990E+00	8.800E+00	3.944	[23, 24]
CCCCCCCCCCCCCC[N+](C)(C)Cc1ccccc1.[Cl-]	0	2.043E+00	2.000E+00	3.301	[23, 24]
CCCCCCCCCCCC[NH2+]CCO.[Cl-]	0	4.405E+01	4.500E+01	4.653	[23, 24]
CCCCCCCCCCCC[NH+]CCO.[Cl-]	0	2.529E+01	3.600E+01	4.556	[23, 24]
CCCCCCCCCCCC[N+]CCO.[Cl-]	0	2.554E+01	2.500E+01	4.398	[23, 24]
CCCCCCCCCC[N+](C)(C)CCCCCCCCCC.[Br-]	0	1.124E+00	1.850E+00	3.267	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCCCCCCCCCC.[Br-]	0	1.720E-01	1.760E-01	2.246	[23, 24]
CCCCCCCCCCCCCCCC(=O)NC(C(=O)[O-])C(C)C.[Na+]	0	1.666E+00	1.900E+00	3.279	[23, 24]
CCCCCCCCCCCCCCCC(=O)NC(CC(C)C)C(=O)[O-].[Na+]	0	1.532E+00	1.500E+00	3.176	[23, 24]
CCCCCCCCCCCS(=O)(=O)[O-].[Li+]	0	1.077E+01	1.100E+01	4.041	[23, 24]
CCCCCCCCCCCS(=O)(=O)[O-].[NH4+]	0	8.711E+00	8.900E+00	3.949	[23, 24]
CCCCCCCCCCCS(=O)(=O)[O-].[K+]	0	9.103E+00	9.300E+00	3.968	[23, 24]
CCCCCCCCCCCOS(=O)(=O)[O-].[Li+]	0	8.711E+00	8.900E+00	3.949	[23, 24]
CCCCCCCC(CC)OS(=O)(=O)[O-].C[N+](C)(C)C	0	5.384E+00	5.500E+00	3.740	[23, 24]
CCCCCCCC(CC)OS(=O)(=O)[O-].CCC[N+](CCC)(CCC)CCC	0	2.248E+00	2.200E+00	3.342	[23, 24]
CCCCCCCCCCCCOCCOS(=O)(=O)[O-].[Na+]	0	4.326E+00	3.900E+00	3.591	[23, 24]
CCCCCCCCCCCCOCCOCCOS(=O)(=O)[O-].[Na+]	0	2.568E+00	2.900E+00	3.462	[23, 24]
CCCCCCCCCCCCCCCCCOCCOCCOCCOCCOCCOS(=O)(=O)[O-].[Na+]	0	2.554E-02	2.500E-02	1.398	[23, 24]
CCCCCCCC(CCCCCC)COCCOCCOCCOCCOCCOS(=O)(=O)[O-].[Na+]	0	8.786E-02	8.600E-02	1.934	[23, 24]
CCCCCOC(=O)CS(=O)(=O)[O-].[Na+]	0	1.808E+02	1.700E+02	5.230	[23, 24]
CCCCCCCOC(=O)CS(=O)(=O)[O-].[Na+]	0	6.743E+01	6.600E+01	4.820	[23, 24]
CCCCCCCCCOC(=O)CS(=O)(=O)[O-].[Na+]	0	2.122E+01	2.200E+01	4.342	[23, 24]
CCCCOC(=O)CC(C(=O)OCCCC)S(=O)(=O)[O-].[Na+]	0	1.175E+02	2.000E+02	5.301	[23, 24]
CCCCCOC(=O)CC(C(=O)OCCCCC)S(=O)(=O)[O-].[Na+]	0	5.188E+01	5.300E+01	4.724	[23, 24]
CCCCC(CC)COC(=O)CC(C(=O)OCC(CC)CCCC)S(=O)(=O)[O-].[Na+]	0	2.554E+00	2.500E+00	3.398	[23, 24]
CCCCCCCCOC(=O)CC(C(=O)OCCCCCCCC)S(=O)(=O)[O-].[Na+]	0	9.297E-01	9.100E-01	2.959	[23, 24]
CCCCCCCCCCCCCC(C(=O)OCC)S(=O)(=O)[O-].[Na+]	0	2.299E+00	2.250E+00	3.352	[23, 24]
CCCCCCCCCCCCCC(C(=O)OCCCC)S(=O)(=O)[O-].[Na+]	0	1.275E+00	1.350E+00	3.130	[23, 24]
CCCCCCOC(=O)CC(C(=O)OCCCCCC)S(=O)(=O)[O-].[Na+]	0	1.462E+01	1.400E+00	3.146	[23, 24]
CCCCCCCCCCCCCCC(C(=O)OC)S(=O)(=O)[O-].[Na+]	0	7.458E-01	7.300E-01	2.863	[23, 24]
CCCCCCCCCC[N+](C)(C)CC(=O)[O-]	0	1.762E+01	1.800E+01	4.255	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CC(=O)[O-]	0	4.237E+00	2.000E+00	3.301	[23, 24]
CCCCCCCCCCCCCC[N+](C)(C)CC(=O)[O-]	0	1.029E+00	2.200E-01	2.342	[23, 24]
CCCCCCCCCCCCCCCC[N+](C)(C)CC(=O)[O-]	0	2.782E-01	2.000E-02	1.301	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCC(=O)[O-]	0	4.503E+00	4.600E+00	3.663	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCCCC(=O)[O-]	0	2.305E+00	2.600E+00	3.415	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCCCCCC(=O)[O-]	0	6.446E-01	1.500E+00	3.176	[23, 24]
CCCCCCCCCCC(C(=O)[O-])[n+]1ccccc1	0	5.090E+00	5.200E+00	3.716	[23, 24]
CCCCCCCCCCCCC(C(=O)[O-])[n+]1ccccc1	0	6.311E-01	6.000E-01	2.778	[23, 24]
CCCCCCCCCCCC[N+](C)(C)CCCS(=O)(=O)[O-]	0	2.936E+00	3.000E+00	3.477	[23, 24]
CCCCCCCCCCCCCC[N+](C)(C)CCCS(=O)(=O)[O-]	0	4.828E-01	3.200E-01	2.505	[23, 24]