Supplementary Information

Identification of structure-biodegradability relationships for ionic liquids - clustering of a dataset based on structural similarity

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List of Tables

Biodegradability data

Data for imidazolium ILs

Table S1: Biodegradability data for imidazolium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Imid_115_0	[Br-].C=1C=CC(C=C=1)n1cc[n+](c1)c1ccccc1	0[1]
Imid_116_0	[Br-].Fc1c(c(F)c(F)c(F)c1F)n1cc[n+](C)c1	0[1]
Imid_36_0	C[N+]1=CN(C=C1)CC#N.[Cl-]	0[2]
Imid_43_0	[Br-].Cn1cc[n+](Cc2ccccc2)c1	0[3]
Imid_45_0	[Br-].C=CC[n+]1ccn(C)c1	0[3]
Imid_74_8	CCN1C=C[N+](=C1)C.[Br-]	8[4]
Imid_76_7	CCN1C(=C([N+](=C1C(C)C)C)C)C.[I-]	7[5]
Imid_77_2	[I-].C[n+]1c(C)c(C)n(CC)c1C	2[5]
Imid_78_6	[I-].Cc1c(C)n(CC)c[n+]1C	6[5]
Imid_1_0	C[N+]1=CN(CCCC)C=C1.[Br-]	0[6–11]
Imid_5_5	C[N+]1=CN(CCCC)C=C1.N#C[N-]C#N	5[6]
Imid_29_1	[N+]1(C)=CN(C=C1)CCCC.[Cl-]	1[12,13]
Imid_31_39	[N+]1(C)=CN(C=C1)CCCCCCCC.[Cl-]	39[12,14,15]
Imid_46_0	CCCC[n+]1ccn(c1)C=C.[I-]	0[3]
Imid_72_31	[N+]1(C)=CN(C=C1)CCCCCC.[Br-]	31[4,9]
Imid_73_41	[N+]1(C)=CN(C=C1)CCCCCCCC.[Br-]	41[9]
Imid_75_26	CCCCCCCCCCN1C=C[N+](=C1)C.[Br-]	26[4]
Imid_79_9	[I-].Cc1c(C)n(CC)c[n+]1C	6[5]
Imid_98_0	[Br-].[Br-].C[n+]1ccn(c1)CCCCCCn1cc[n+](C)c1	0[16]
Imid_100_0	[Br-].[Br-].CCCCCC[n+]1cn(CCn2cc[n+](c2)CCCCCC)cc1	0[16]
Imid_104_0	[Br-].Cc1ccc(cc1)n1cc[n+](c1)CCCC	0[17]
Imid_117_0	[Cl-].C[n+]1ccn(CCCCCCCCCCCCCCCC)c1	0[1,18]
Imid_146_10	CCCCCCCCCCCCN1C=C[N+](=C1)C.[Br-]	10[19]
Imid_185_9	[Br-].[Br-].CCCCCCCCCCCCn1cc[n+](c1)CCCC[n+]1ccn(CCCCCCCCCCCC)c1	9[19]
Imid_186_13	[Br-].[Br-].CCCCCCCCCCCCCCn1cc[n+](c1)CCCC[n+]1ccn(CCCCCCCCCCCCCC)c1	13[19]

Imid_187_18	[Br-].[Br-].CCCCCCCCCCCCCCCCn1cc[n+](c1)CCCC[n+]1ccn(CCCCCCCCCCCCCCCC)c1	18[19]
Imid_188_18	CCCCCCCCCCCCCCN1C=C[N+](=C1)C.[Br-]	18[19]
Imid_189_20	CCCCCCCCCCCCCCCCCN1C=C[N+](=C1)C.[Br-]	20[19]
Imid_13_0	[Br-].C[n+]1ccn(CC(=O)NCCCC)c1	0[7]
Imid_246_0	CN1C=C[N+](C(C(NCCCC)=O)C2=CC=CC=C2)=C1.[Br-]	0[20]
Imid_190_32	CCCCn1cc[n+](C)c1.[O-]C(=O)C1CCCN1	32[21]
Imid_191_47	CCCCn1cc[n+](C)c1.CC(C)C(N)C([O-])=O	47[21]
Imid_192_33	CCCCn1cc[n+](C)c1.[O-]C(=O)CN	33[21]
Imid_193_19	CCCCn1cc[n+](C)c1.[O-]C(=O)C(N)CS	19[21]
Imid_194_25	CCCCn1cc[n+](C)c1.[O-]C(=O)C(N)Cc1c[NH]cn1	25[21]
Imid_195_30	CCCCn1cc[n+](C)c1.[O-]C(=O)C(N)Cc1ccccc1	30[21]
Imid_196_46	CCCCn1cc[n+](C)c1.[O-]C(=O)C(N)CC(=O)O	46[21]
Imid_197_16	SCC(N)C([O-])=O.C[n+]1ccn(CC)c1	16[21]
Imid_198_17	[O-]C(=O)C(N)CS.C[n+]1ccn(CCCCCC)c1	17[21]
Imid_234_47	[Br-].O=C(C[n+]1ccn(C)c1)N[C@@H](Cc1ccccc1)C(=O)OCC	47[22,23]
Imid_235_56	O=C([C@H](CC1=CC=CC=C1)NC(C[N+]2=CN(C=C2)C)=O)OCCCC.[Br-]	56[23,24]
Imid_236_51	O=C([C@H](CC1=CC=CC=C1)NC(C[N+]2=CN(C=C2)C)=O)OCCCCCC.[Br-]	51[23]
Imid_237_48	CN1C=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCCCCCCCC)=O)=O)=C1.[Br-]	48[23]
Imid_238_44	CN1C=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCCCCCCCCCC)=O)=O)=C1.[Br-]	44[23,25]
Imid_239_15	CN1C=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCCCCCCCCCCCC)=O)=O)=C1.[Br-]	15[23]
Imid_240_40	CCOC([C@H](CC1=CC=CC=C1)NC(CN2C=C[N+](CC(N[C@@H](CC3=CC=CC=C3)C(OCC)=O)=O)=C2)=O)=O.[Br-]	40[22,26]
Imid_241_64	[Br-].C[n+]1ccn(CC(=O)NC(Cc2ccccc2)C(=O)NC(CC(C)C)C(=O)OC)c1	64[24]
Imid_242_40	CCOC([C@H](CC1=CC=C(O)C=C1)NC(C[N+]2=CN(C)C=C2)=O)=O.[Br-]	40[22]
Imid_168_2	[Br-].O=C(c1cn(CC(=O)OCC)c[n+]1Cc1ccccc1)N1CCCC1	2[27]
Imid_169_2	[Br-].O=C(c1n(CC(=O)OCC)c[n+](Cc2ccccc2)c1C(=O)N1CCCC1)N1CCCC1	2[27]
Imid_14_0	[Br-].C[n+]1ccn(CC(=O)N(C)CCCC)c1	0[7]
Imid_15_0	[Br-].C[n+]1ccn(CC(=O)N(CC)CC)c1	0[7]
Imid_158_3	[Br-].O=C(Cn1cc[n+](C)c1)N1CCCC1	3[27]
Imid_159_0	[Br-].O=C(Cn1cc[n+](Cc2ccccc2)c1)N1CCCC1	0[27]
Imid_160_3	[Br-].O=C(Cn1cc[n+](C)c1C)N1CCCC1	3[27]

Imid_161_12	[Br-].O=C(Cn1cc[n+](C)c1C(N)=O)N1CCCC1	12[27]
Imid_162_14	O=C(Cn1cc[n+](C)c1C(N)=O)N1CCCC1.F[B-](F)(F)F	14[27]
Imid_3_4	C[N+]1=CN(CCCC)C=C1.F[B-](F)(F)F	4[6–8,28,29]
Imid_4_3	C[N+]1=CN(CCCC)C=C1.F[P-](F)(F)(F)(F)F	3[6,7,13,28]
Imid_70_0	C[n+]1ccn(CCC)c1.F[P-](F)(F)(F)(F)F	0[2]
Imid_249_21	[B-](F)(F)(F)F.CCCCCCCCCCN1C=C[N+](=C1)C	21[11]
Imid_18_16	F[B-](F)(F)F.O=C(OCCC)Cn1cc[n+](C)c1	16[6]
Imid_19_16	F[P-](F)(F)(F)(F)F.O=C(OCCC)Cn1cc[n+](C)c1	16[6]
Imid_54_4	Cn1cc[n+](CCCC)c1.[O-]P(=O)(OCCCC)OCCCC	4[3]
Imid_153_3	CN1C=CN(CC=C)[CH+]1.FC(F)(F)C(C(F)(F)F)O[Al-](OC(C(F)(F)F)C(F)(F)F)(OC(C(F)(F)F)C(F)(F)F)OC(C(F)(F)F)C(F)(F)F	3[30]
Imid_154_0	CN1C=CN(CCCC)[C+]1C.FC(F)(F)C(C(F)(F)F)O[Al-](OC(C(F)(F)F)C(F)(F)F)(OC(C(F)(F)F)C(F)(F)F)OC(C(F)(F)F)C(F)(F)F	0[30]
Imid_155_2	CN1C=CN(CCCCCC)[CH+]1.FC(F)(F)C(C(F)(F)F)O[Al-](OC(C(F)(F)F)C(F)(F)F)(OC(C(F)(F)F)C(F)(F)F)OC(C(F)(F)F)C(F)(F)F	2[30]
Imid_157_14	COC(=O)Cn1cc[n+](C)c1.F[B-](F)(F)F	14[27]
Imid_165_35	Cn1cc[n+](C)c1C(=O)OCC(C)C.F[B-](F)(F)F	35[27]
Imid_167_5	F[B-](F)(F)F.O=C(OCC)c1cn(CC(=O)OCC)c[n+]1C	5[27]
Imid_171_6	F[B-](F)(F)F.O=C(OC)c1c([n+](cn1CC(=O)OCC)Cc1ccccc1)C(=O)OC	6[27]
Imid_172_31	F[B-](F)(F)F.O=C(OC)c1c([n+](C)cn1CC(=O)OCC)C(=O)OC	31[27]
Imid_173_3	C[n+]1cn(C)c(c1C(=O)OC)C(=O)OC.F[B-](F)(F)F	3[27]
Imid_179_100	[Cl-].[Cl-].CCCCCCCCCCCC(=O)OCCC[n+]1ccn(CCCCn2cc[n+](c2)CCCOC(=O)CCCCCCCCCCC)c1	100[19]
Imid_180_100	[Cl-].[Cl-].CCCCCCCCCCCCCC(=O)OCCC[n+]1ccn(CCCCn2cc[n+](c2)CCCOC(=O)CCCCCCCCCCCCC)c1	100[19]
Imid_181_100	[Cl-].[Cl-].CCCCCCCCCCCCCCCC(=O)OCCC[n+]1ccn(CCCCn2cc[n+](c2)CCCOC(=O)CCCCCCCCCCCCCC)c1	100[19]
Imid_182_50	[Br-].[Br-].Cn1cc[n+](CC(COC(=O)CCCCCCCCCCC)(C[n+]2ccn(C)c2)COC(=O)CCCCCCCCCCC)c1	50[19]
Imid_183_53	[Br-].[Br-].Cn1cc[n+](CC(COC(=O)CCCCCCCCCCCCC)(C[n+]2ccn(C)c2)COC(=O)CCCCCCCCCCCCC)c1	53[19]
Imid_184_65	[Br-].[Br-].Cn1cc[n+](CC(COC(=O)CCCCCCCCCCCCCC)(C[n+]2ccn(C)c2)COC(=O)CCCCCCCCCCCCC)c1	65[19]
Imid_10_26	[Br-].O=C(OCCCC)Cn1cc[n+](C)c1	26[7]
Imid_11_24	[Br-].O=C(OCCCCCC)Cn1cc[n+](C)c1	24[7]
Imid_12_27	[Br-].O=C(OCCCCCCCC)Cn1cc[n+](C)c1	27[7]
Imid_16_21	[Br-].O=C(OCCC)Cn1cc[n+](C)c1	21[6–8]
Imid_22_23	[Br-].O=C(OCCC)Cn1cc[n+](C)c1C	23[8]

Imid_23_32	[Br-].O=C(OCCCCC)Cn1cc[n+](C)c1	32[3,7,8]
Imid_24_33	[Br-].O=C(OCCCCC)Cn1cc[n+](C)c1C	33[8]
Imid_44_23	[I-].Cn1cc[n+](CCCCOC(C)=O)c1	23[3]
Imid_109_7	[Br-].O=C(OCC)c1ccc(cc1)n1cc[n+](c1)CCCC	7[17]
Imid_110_8	[Br-].O=C(OCC)c1ccc(cc1)n1cc[n+](c1)CCCCCC	8[17]
Imid_245_27	CN1C=C[N+](C(C(OCCCC)=O)C2=CC=CC=C2)=C1.[Br-]	27[20]
Imid_20_34	N#C\N=C=[N-].O=C(OCCC)Cn1cc[n+](C)c1	34[6]
Imid_229_29	N#CCn1cc[n+](CCOCC)c1.N#C[N-]C#N	29[31]
Imid_230_23	N#CCn1cc[n+](CCOCC)c1.FC(F)(F)C([O-])=O	23[31]
Imid_247_62	CCCCn1cc[n+](C)c1.CCCCCCCCCCCC(=O)N(C)CC([O-])=O	62[32]
Imid_248_57	O=C([O-])CN(C)C(=O)CCCCCCCCCCC.C[n+]1ccn(CC)c1	57[32]
Imid_53_17	Cn1cc[n+](CCCC)c1.[O-]C(=O)C(C)O	17[3]
Imid_80_25	CCCCn1cc[n+](C)c1.CC(=O)CCC([O-])=O	25[33]
Imid_112_0	O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.C[n+]1ccn(CC)c1	0[34]
Imid_120_9	O=C([O-])C.C[n+]1ccn(CC)c1	9[35]
Imid_42_0	[Br-].OCC[n+]1ccn(C)c1	0[3]
Imid_114_0	C[n+]1ccn(CCO)c1.FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C([O-])=O	0[34]
Imid_8_21	[Br-].O=C(OCC)Cn1cc[n+](C)c1	21[7]
Imid_156_14	[Br-].COC(=O)Cn1cc[n+](C)c1	14[7,27]
Imid_163_17	[Br-].COC(=O)Cn1cc[n+](C)c1C(N)=O	17[27]
Imid_164_30	[I-].Cn1cc[n+](C)c1C(=O)OCC(C)C	30[27]
Imid_166_10	[Br-].O=C(OCC)c1cn(CC(=O)OCC)c[n+]1C	10[27]
Imid_170_24	[Br-].O=C(OC)c1c([n+](cn1CC(=O)OCC)Cc1ccccc1)C(=O)OC	24[27]
Imid_174_12	[I-].C[n+]1cn(C)c(c1C(=O)OC)C(=O)OC	12[27]
Imid_243_5	CN1C=C[N+](C(C(OC)=O)C2=CC=CC=C2)=C1.[Br-]	5[20]
Imid_244_20	CN1C=C[N+](C(C2=CC=CC=C2)C(OCC)=O)=C1.[Br-]	20[20]
Imid_250_0	[Br-].OC(=O)C[n+]1ccn(C)c1	0[23]
Imid_122_35	[Cl-].[Cl-].[Cl-].[Cl-].CCCC[n+]1ccn(c1)CC(=O)OCC(COC(=O)Cn1cc[n+](c1)CCCC)(COC(=O)Cn1cc[n+](CCCC)c1)COC(=O)Cn1cc[n+](CCCC)c1	35[36]
Imid_123_39	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCC[n+]1ccn(c1)CC(=O)OCC(COC(=O)Cn1cc[n+](c1)CCCCCC)(COC(=O)Cn1cc[n+](CCCCCC)c1)COC(=O)Cn1cc[n+](CCCCCC)c1	39[36]

Imid_124_49	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCC[n+]1ccn(c1)CC(=O)OCC(COC(=O)Cn1cc[n+](c1)CCCCCCCC)(COC(=O)Cn1cc[n+](CCCCCCCC)c1)COC(=O)Cn1cc[n+](CCCCCCCC)c1	49[36]
Imid_125_52	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCCCC[n+]1ccn(c1)CC(=O)OCC(COC(=O)Cn1cc[n+](c1)CCCCCCCCCC)(COC(=O)Cn1cc[n+](CCCCCCCCCC)c1)COC(=O)Cn1cc[n+](CCCCCCCCCC)c1	52[36]
Imid_126_53	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCCCCCC[n+]1ccn(c1)CC(=O)OCC(COC(=O)Cn1cc[n+](c1)CCCCCCCCCCCC)(COC(=O)Cn1cc[n+](CCCCCCCCCCCC)c1)COC(=O)Cn1cc[n+](CCCCCCCCCCCC)c1	53[36]
Imid_134_27	[Cl-].[Cl-].[Cl-].CCCC[n+]1ccn(c1)CC(=O)OCC(C)(COC(=O)Cn1cc[n+](c1)CCCC)COC(=O)Cn1cc[n+](CCCC)c1	27[37]
Imid_135_36	[Cl-].[Cl-].[Cl-].CCCCCC[n+]1ccn(c1)CC(=O)OCC(C)(COC(=O)Cn1cc[n+](c1)CCCCCC)COC(=O)Cn1cc[n+](CCCCCC)c1	36[37]
Imid_136_47	[Cl-].[Cl-].[Cl-].CCCCCCCC[n+]1ccn(c1)CC(=O)OCC(C)(COC(=O)Cn1cc[n+](c1)CCCCCCCC)COC(=O)Cn1cc[n+](CCCCCCCC)c1	47[37]
Imid_137_45	[Cl-].[Cl-].[Cl-].CCCCCCCCCC[n+]1ccn(c1)CC(=O)OCC(C)(COC(=O)Cn1cc[n+](c1)CCCCCCCCCC)COC(=O)Cn1cc[n+](CCCCCCCCCC)c1	45[37]
Imid_138_51	[Cl-].[Cl-].[Cl-].CCCCCCCCCCCC[n+]1ccn(c1)CC(=O)OCC(C)(COC(=O)Cn1cc[n+](c1)CCCCCCCCCCCC)COC(=O)Cn1cc[n+](CCCCCCCCCCCC)c1	51[37]
Imid_128_28	[Cl-].[Cl-].[Cl-].CCCC[n+]1cn(CC(=O)OCC(COC(=O)Cn2c[n+](CCCC)c3ccccc32)(COC(=O)Cn2c[n+](CCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCC)c3ccccc32)c2ccccc21	28[36]
Imid_129_34	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCC[n+]1cn(CC(=O)OCC(COC(=O)Cn2c[n+](CCCCCC)c3ccccc32)(COC(=O)Cn2c[n+](CCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCC)c3ccccc32)c2ccccc21	34[36]
Imid_130_42	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCC[n+]1cn(CC(=O)OCC(COC(=O)Cn2c[n+](CCCCCCCC)c3ccccc32)(COC(=O)Cn2c[n+](CCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCC)c3ccccc32)c2ccccc21	42[36]
Imid_140_22	[Cl-].[Cl-].[Cl-].CCCC[n+]1cn(CC(=O)OCC(C)(COC(=O)Cn2c[n+](CCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCC)c3ccccc32)c2ccccc21	22[37]
Imid_141_27	[Cl-].[Cl-].[Cl-].CCCCCC[n+]1cn(CC(=O)OCC(C)(COC(=O)Cn2c[n+](CCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCC)c3ccccc32)c2ccccc21	27[37]
Imid_142_36	[Cl-].[Cl-].[Cl-].CCCCCCCC[n+]1cn(CC(=O)OCC(C)(COC(=O)Cn2c[n+](CCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCC)c3ccccc32)c2ccccc21	36[37]
Imid_143_40	[Cl-].[Cl-].[Cl-].CCCCCCCCCC[n+]1cn(CC(=O)OCC(C)(COC(=O)Cn2c[n+](CCCCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCCCC)c3ccccc32)c2ccccc21	40[37]
Imid_144_45	[Cl-].[Cl-].[Cl-].CCCCCCCCCCCC[n+]1cn(CC(=O)OCC(C)(COC(=O)Cn2c[n+](CCCCCCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCCCCCC)c3ccccc32)c2ccccc21	45[37]
Imid_127_22	[Cl-].[Cl-].[Cl-].[Cl-].O=C(Cn1cc[n+](Cc2ccccc2)c1)OCC(COC(=O)Cn1cc[n+](c1)Cc1ccccc1)(COC(=O)Cn1cc[n+](Cc2ccccc2)c1)COC(=O)Cn1cc[n+](Cc2ccccc2)c1	22[36]
Imid_133_22	[Cl-].[Cl-].[Cl-].[Cl-].O=C(Cn1c[n+](Cc2ccccc2)c2ccccc21)OCC(COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21)(COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21)COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21	22[36]
Imid_139_20	[Cl-].[Cl-].[Cl-].CC(COC(=O)Cn1cc[n+](c1)Cc1ccccc1)(COC(=O)Cn1cc[n+](Cc2ccccc2)c1)COC(=O)Cn1cc[n+](Cc2ccccc2)c1	20[37]
Imid_145_16	[Cl-].[Cl-].[Cl-].CC(COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21)(COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21)COC(=O)Cn1c[n+](Cc2ccccc2)c2ccccc21	16[37]
Imid_55_42	CCCC[n+]1ccn(C)c1.O=C1[N-]S(=O)(=O)c2ccccc12	42[3]
Imid_56_61	O=C(OCCCCC)C[n+]1ccn(C)c1.O=C1[N-]S(=O)(=O)c2ccccc12	61[3]
Imid_6_5	CCCCN1C=C[N+](=C1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	5[6]
Imid_21_25	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.O=C(OCCC)Cn1cc[n+](C)c1	25[6]
Imid_231_65	N#CCn1cc[n+](CCOCC)c1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	65[31]

Imid_232_62	N#CCn1cc[n+](CCOCCOC)c1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	62[31]
Imid_233_62	N#CCn1cc[n+](CCOCCOCCOC)c1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	62[31]
Imid_51_8	Cn1cc[n+](CCCC)c1.[O-]S(C)(=O)=O	8[3]
Imid_111_0	C[n+]1ccn(CC)c1.FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S([O-])(=O)=O	0[34]
Imid_113_0	C[n+]1ccn(CCO)c1.FC(F)(F)C(F)(F)C(F)(F)C(F)(F)S([O-])(=O)=O	0[34]
Imid_2_33	CCCCCCCCOS(=O)(=O)[O-].CCCCN1C=C[N+](=C1)C	33[3,6]
Imid_47_38	Cn1cc[n+](Cc2ccccc2)c1.[O-]S(=O)(=O)OCCCCCCCCC	38[3]
Imid_48_44	C=CC[n+]1ccn(C)c1.[O-]S(=O)(=O)OCCCCCCCCC	44[3]
Imid_49_43	C=Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCCCC	43[3]
Imid_57_34	Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCC	34[3]
Imid_58_36	Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	36[3]
Imid_60_47	Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCC	47[3]
Imid_61_54	Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCCC	54[3]
Imid_62_58	Cn1cc[n+](CCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCCCC	58[3]
Imid_63_30	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCC	30[3]
Imid_64_33	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCCC	33[3]
Imid_65_38	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	38[3]
Imid_66_36	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCCC	36[3]
Imid_67_44	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCC	44[3]
Imid_68_49	Cn1cc[n+](CCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCCC	49[3]
Imid_17_49	[O-]S(=O)(=O)OCCCCCCCC.O=C(OCCC)Cn1cc[n+](C)c1	49[6,8]
Imid_25_55	[O-]S(=O)(=O)OCCCCCCCC.O=C(OCCC)Cn1cc[n+](C)c1C	55[8]
Imid_26_60	[O-]S(=O)(=O)OCCCCCCCC.O=C(OCCCCC)Cn1cc[n+](C)c1	60[3,8,38]
Imid_27_56	[O-]S(=O)(=O)OCCCCCCCC.O=C(OCCCCC)Cn1cc[n+](C)c1C	56[8]
Imid_50_54	Cn1cc[n+](CCCCOC(C)=O)c1.[O-]S(=O)(=O)OCCCCCCCC	54[3]
Imid_52_34	Cn1cc[n+](CC(=O)OCCCCC)c1.[O-]S(C)(=O)=O	34[3]
Imid_69_72	Cn1cc[n+](CC(=O)OCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCCCCC	72[3]
Imid_81_62	Cn1cc[n+](CC(=O)OCCOCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	62
Imid_82_59	Cn1cc[n+](CC(=O)OCCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	59[38]
Imid_83_65	Cn1cc[n+](CC(=O)OCCOCCOCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	65[38]

Imid_84_63	Cn1cc[n+](CC(=O)OCCOCCOCCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	63[38]
Imid_85_59	Cn1cc[n+](CC(=O)OCCOCCOC)c1.[O-]S(=O)(=O)OCCCCCCCC	59[38]
Imid_86_58	Cn1cc[n+](CC(=O)OCCOCCOCC)c1.[O-]S(=O)(=O)OCCCCCCCC	58[38]
Imid_87_60	Cn1cc[n+](CC(=O)OCCOCCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	60[38]
Imid_88_58	Cn1cc[n+](CC(=O)OCCOCC)c1.[O-]S(=O)(=O)OCCCCCCCC	58[38]
Imid_89_58	Cn1cc[n+](CC(=O)OCCOC)c1.[O-]S(=O)(=O)OCCCCCCCC	58[38]
Imid_90_62	Cc1[n+](CC(=O)OCCOCCCC)ccn1C.[O-]S(=O)(=O)OCCCCCCCC	62[38]
Imid_91_58	Cc1[n+](CC(=O)OCCOCCOC)ccn1C.[O-]S(=O)(=O)OCCCCCCCC	58[38]
Imid_92_38	O=C(C[n+]1ccn(C)c1)N1CCCC1.[O-]S(=O)(=O)OCCCCCCCC	38[38]
Imid_93_35	O=C(C[n+]1ccn(C)c1C)N1CCCC1.[O-]S(=O)(=O)OCCCCCCCC	35[38]
Imid_94_25	O=C(C[n+]1ccn(C)c1)N(CCOC)CCOC.[O-]S(=O)(=O)OCCCCCCCC	25[38]
Imid_131_44	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCCCC[n+]1cn(CC(=O)OCC(COC(=O)Cn2c[n+](CCCCCCCCCC)c3ccccc32)(COC(=O)Cn2c[n+](CCCCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCCCC)c3ccccc32)c2ccccc21	44[36]
Imid_132_47	[Cl-].[Cl-].[Cl-].[Cl-].CCCCCCCCCCCC[n+]1cn(CC(=O)OCC(COC(=O)Cn2c[n+](CCCCCCCCCCCC)c3ccccc32)(COC(=O)Cn2c[n+](CCCCCCCCCCCC)c3ccccc32)COC(=O)Cn2c[n+](CCCCCCCCCCCC)c3ccccc32)c2ccccc21	47[36]

Data for pyridinium ILs

Table S2: Biodegradability data for pyridinium ILs.

IL (cation_number_biodegradation rate)	SMILES	biodegradation rate in %
Pyri_1_69	[Br-].OC(=O)C[n+]1ccccc1	69[26]
Pyri_2_5	COC1=CC=C[N+](CC(O)=O)=C1.[Br-]	5[26]
Pyri_3_7	CN(C1=CC=[N+](CC(O)=O)C=C1)C.[Br-]	7[26]
Pyri_85_54	O=C(N[C@H](C(OCC)=O)CC1=CC=CC=C1)C[N+]2=CC=CC=C2.[Br-]	54[20,22,23,26]
Pyri_91_47	COC1=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCC)=O)=O)=CC=C1.[Br-]	47[22,26]
Pyri_92_32	CCOC(C1=C[N+](CC(N[C@H](C(OCC)=O)CC2=CC=CC=C2)=O)=CC=C1)=O.[Br-]	32[26]
Pyri_93_37	OC(C1=CC=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCC)=O)=O)=C1)=O.[Br-]	37[26]
Pyri_94_56	CCOC(C1=CC=C[N+](CC(N[C@@H](CC2=CC=CC=C2)C(O)=O)=O)=C1)=O.[Br-]	56[26]
Pyri_95_33	CN(C)C1=CC=[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCC)=O)=O)C=C1.[Br-]	33[26]
Pyri_96_49	CCOC([C@H](CC1=CC=C(O)C=C1)NC(C[N+]2=CC=CC=C2)=O)=O.[Br-]	49[22]
Pyri_97_46	CCOC([C@H](CC1=CC=C(O)C=C1)NC(C[N+]2=CC(OC)=CC=C2)=O)=O.[Br-]	46[22]

Pyri_98_31	CCOC([C@H](CC1=CC=C(O)C=C1)NC(C[N+]2=CC=CC(C(OCC)=O)=C2)=O)=O.[Br-]	31[22]
Pyri_86_49	CCCCOC([C@@H](NC(C[N+]1=CC=CC=C1)=O)CC2=CC=CC=C2)=O.[Br-]	49[23]
Pyri_87_46	O=C([C@H](CC1=CC=CC=C1)NC(C[N+]2=CC=CC=C2)=O)OCCCCCC.[Br-]	46[23]
Pyri_88_52	O=C(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCC)=O)C[N+]2=CC=CC=C2.[Br-]	52[23]
Pyri_89_27	O=C(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCCCC)=O)C[N+]2=CC=CC=C2.[Br-]	27[23,25]
Pyri_90_4	O=C(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCCCCCC)=O)C[N+]2=CC=CC=C2.[Br-]	4[23]
Pyri_102_1	O=C(NCCCC)C(C1=CC=CC=C1)[N+]2=CC=CC=C2.[Br-]	1[20]
Pyri_109_4	[Br-].O\N=C\c1cc[n+](CC(=O)NCCCCCCCC)cc1	4[39]
Pyri_110_9	[Br-].O\N=C\c1cc[n+](CC(=O)NC(C)C(=O)NCCCCCCCC)cc1	9[39]
Pyri_111_24	[Br-].O\N=C\c1cccc[n+]1CC(=O)NC(Cc1ccccc1)C(=O)NCCCCCCCC	24[39]
Pyri_112_20	[Br-].O\N=C\c1ccc[n+](CC(=O)NC(Cc2ccccc2)C(=O)NCCCCCCCC)c1	20[39]
Pyri_113_25	[Br-].O\N=C\c1cc[n+](CC(=O)NC(Cc2ccccc2)C(=O)NCCCCCCCC)cc1	25[39]
Pyri_5_1	[n+]1(ccccc1)CCCC.[Cl-]	1[12,13]
Pyri_33_0	C1=CC=[N+](C=C1)CC#N.[Cl-]	0[2]
Pyri_35_1	CCC[N+]1=CC=CC=C1.[Br-]	1[2]
Pyri_36_0	[n+]1(ccccc1)CCCC.[Br-]	0[40]
Pyri_39_3	F[P-](F)(F)(F)(F)F.CCCC[n+]1ccccc1	3[40]
Pyri_40_3	CCCC[N+]1=CC=CC(=C1)C.[Br-]	3[9,10,40]
Pyri_42_9	[n+]1(ccccc1)CCCCCCCCCC.[Br-]	9[40]
Pyri_43_0	[n+]1(ccccc1)CCCCCCCCCCCCCCCC.[Br-]	0[40]
Pyri_51_90	CCCCCCCC[N+]1=CC=CC(=C1)C.[Br-]	90[10,41]
Pyri_52_10	CCCCCC[N+]1=CC=CC(=C1)C.[Br-]	10[41]
Pyri_78_2	C1=CC=C(C=C1)C[N+]2=CC=CC=C2.[Br-]	2[27]
Pyri_80_0	CCCC[N+]1=CC=CC(=C1)C.C(=[N-])=NC#N	0[29]
Pyri_108_0	CCCC[N+]1=CC=C(C=C1)C.[Cl-]	0[11]
Pyri_24_88	[n+]1(ccccc1)CC(=O)OCC.[Br-]	88[40,42]
Pyri_28_76	[n+]1(cc(C(=O)OCCCC)ccc1)C.[I-]	76[40,42]
Pyri_45_88	[n+]1(ccccc1)CC(=O)OCC.[P-](F)(F)(F)(F)(F)F	88[40]
Pyri_46_75	[n+]1(cc(C(=O)OCCCC)ccc1)C.[P-](F)(F)(F)(F)(F)F	75[40]
Pyri_60_37	CC[n+]1cccc(C)c1.FC(F)(F)C(F)(F)C(F)(F)C(F)(F)C([O-])=O	37[34]

Pyri_79_25	CCOC(=O)C1=C[N+](=CC=C1)CC2=CC=CC=C2.[Br-]	25[27]
Pyri_99_8	O=C(OC)C(C1=CC=CC=C1)[N+]2=CC=CC=C2.[Br-]	8[20]
Pyri_100_16	O=C(OCC)C(C1=CC=CC=C1)[N+]2=CC=CC=C2.[Br-]	16[20]
Pyri_101_21	O=C(OCCCC)C(C1=CC=CC=C1)[N+]2=CC=CC=C2.[Br-]	21[20]
Pyri_103_22	COC1=CC=C[N+](C(C(OCCCC)=O)C2=CC=CC=C2)=C1.[Br-]	22[20]
Pyri_104_31	CCOC(C1=CC=C[N+](C(C(OCCCC)=O)C2=CC=CC=C2)=C1)=O.[Br-]	31[20]
Pyri_105_63	CCCCCCCCCCCC(=O)N(C)CC([O-])=O.CCCC[n+]1ccccc1	63[32]
Pyri_106_78	CCCCCCCCCCCC(=O)N(C)CC([O-])=O.CCCCCC[n+]1ccccc1	78[32]
Pyri_107_80	Cc1cc[n+](CCCCCCCC)cc1C.CCCCCCCCCCCC(=O)N(C)CC([O-])=O	80[32]
Pyri_73_40	[n+]1(cc(O)ccc1)COCCC.[Cl-]	40[43]
Pyri_74_44	[n+]1(cc(O)ccc1)COCCCCCCC.[Cl-]	44[43]
Pyri_75_48	[n+]1(cc(O)ccc1)COCCCCCCCCCCC.[Cl-]	48[43]
Pyri_76_25	[Cl-].Oc1ccc[n+](COCCCCCCCCCCCCCCCCCC)c1	25[43]
Pyri_20_5	[Cl-].[Cl-].O(CC[n+]1ccccc1)COCC[n+]1ccccc1	5[44]
Pyri_22_3	F[P-](F)(F)(F)(F)F.F[P-](F)(F)(F)(F)F.O(CC[n+]1ccccc1)COCC[n+]1ccccc1	3[44]
Pyri_32_51	C1=CC=[N+](C=C1)CCO.[Cl-]	51[2]
Pyri_34_65	c1cc[n+](cc1)CCO.[I-]	65[2]
Pyri_15_32	CCCCCCCCOS(=O)(=O)[O-].CCCC[n+]1cccc(c1)COC	32[44]
Pyri_16_31	CCCCCCCC[n+]1cccc(c1)COC.CCCCCCCCOS(=O)(=O)[O-]	31[44]
Pyri_17_36	CCCCCCCCOS(=O)(=O)[O-].CCCC[n+]1cccc(c1)COCC	36[44]
Pyri_18_47	CCCCCCCCOS(=O)(=O)[O-].CCOC(=O)C[n+]1cccc(c1)COC	47[44]
Pyri_19_51	COCc1ccc[n+](CC(=O)OCCCCC)c1.[O-]S(=O)(=O)OCCCCCCCC	51[44]
Pyri_25_89	[n+]1(ccccc1)CC(=O)OCC.[O-]S(=O)(=O)OCCCCCCCC	89[40,42]
Pyri_26_75	[n+]1(cc(C(=O)OCCCC)ccc1)C.[O-]S(=O)(=O)OCCCCCCCC	75[40,42]
Pyri_30_30	CCCCCCCCOS(=O)(=O)[O-].CCCCNC(=O)c1ccc[n+](c1)CCCC	30[40,42]
Pyri_37_40	CCCCCCCCS(=O)(=O)[O-].CCCC[N+]1=CC=CC=C1	40[40]
Pyri_41_37	CCCCCCCCOS(=O)(=O)[O-].CCCC[n+]1cccc(c1)C	37[40]
Pyri_47_82	[O-]S(=O)(=O)OCCCCCCCC.O=C(OCCCC)c1ccc[n+](CCCC)c1	82[40,42]
Pyri_61_24	[n+]1(cc(O)ccc1)COCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	24[43]
Pyri_62_22	[n+]1(cc(O)ccc1)COCCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	22[43]

Pyri_63_39	[n+]1(cc(O)ccc1)COCCCCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	39[43]
Pyri_64_41	[n+]1(cc(O)ccc1)COCCCCCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	41[43]
Pyri_65_49	[n+]1(cc(O)ccc1)COCCCCCCCCCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	49[43]
Pyri_66_32	[n+]1(cc(O)ccc1)COCCCCCCCCCCCCCCCCCC.[N-]1C(=O)C=C(C)OS1(=O)=O	32[43]
Pyri_67_43	[n+]1(cc(O)ccc1)COCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	43[43]
Pyri_68_13	[n+]1(cc(O)ccc1)COCCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	13[43]
Pyri_69_31	[n+]1(cc(O)ccc1)COCCCCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	31[43]
Pyri_70_32	[n+]1(cc(O)ccc1)COCCCCCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	32[43]
Pyri_71_72	[n+]1(cc(O)ccc1)COCCCCCCCCCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	72[43]
Pyri_72_20	[n+]1(cc(O)ccc1)COCCCCCCCCCCCCCCCCCC.[N-]1C(=O)c2ccccc2S1(=O)=O	20[43]
Pyri_11_71	CCCCOC(=O)c1ccc[n+](c1)CCO.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	71[44]
Pyri_12_62	c1cc[n+](cc1)CCO.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	62[44]
Pyri_13_1	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCOC[n+]1cccc(CCCC)c1	1[44]
Pyri_14_6	COCc1ccc[n+](c1)CCO.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	6[44]
Pyri_21_4	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.O(CC[n+]1ccccc1)COCC[n+]1ccccc1	4[44]
Pyri_23_3	CCCNC(=O)OCC[n+]1ccccc1.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	3[44]
Pyri_29_68	[n+]1(cc(C(=O)OCCCC)ccc1)C.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	68[40,42]
Pyri_38_0	CCCC[N+]1=CC=CC=C1.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	0[40]
Pyri_44_64	[n+]1(ccccc1)CC(=O)OCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	64[40]
Pyri_53_0	C=CC[n+]1ccccc1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	0[45]
Pyri_54_1	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.c1ccccc1C[n+]1ccccc1	1[45]
Pyri_55_0	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CC(C)N(CC[n+]1ccccc1)C(C)C	0[45]
Pyri_56_3	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCN(CC)Cc1ccc[n+](CCCC)c1	3[45]
Pyri_57_3	CCCC[N+]1=CC=CC(=C1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	3[45]
Pyri_58_60	OC(=O)Cc1ccc[n+](CCCC)c1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	60[45]

Data for QACs

Table S3: Biodegradability data for QACs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
QAC_171_92	[Cl-].O=C(OCC)[C@@H]([NH3+])Cc1ccccc1	92[23]
QAC _172_99	[Cl-].O=C(OCCCC)[C@@H]([NH3+])Cc1ccccc1	99[23]
QAC _173_85	[Cl-].O=C(OCCCCCC)[C@@H]([NH3+])Cc1ccccc1	85[23]
QAC_174_79	[Cl-].O=C(OCCCCCCCC)[C@@H]([NH3+])Cc1ccccc1	79[23]
QAC_175_50	[Cl-].O=C(OCCCCCCCCCC)[C@@H]([NH3+])Cc1ccccc1	50[23]
QAC_176_65	[Cl-].O=C(OCCCCCCCCCCCC)[C@@H]([NH3+])Cc1ccccc1	65[23]
QAC_177_67	[Cl-].O=C(OCCCCCCCCCCCCCC)[C@@H]([NH3+])Cc1ccccc1	67[23]
QAC_178_52	[Cl-].O=C(OCCCCCCCCCCCCCCCC)[C@@H]([NH3+])Cc1ccccc1	52[23]
QAC_20_86	[O-]C=O.[NH3+]CCO	86[12]
QAC_21_95	CCCC(=O)[O-].[NH3+]CCO	95[12]
QAC_22_13	O=C[O-].OCC[NH2+]CCO	13[12]
QAC_23_69	O=C([O-])C.OCC[NH2+]CCO	69[12]
QAC_24_68	O=C([O-])CC.OCC[NH2+]CCO	68[12]
QAC_25_78	O=C([O-])CCC.OCC[NH2+]CCO	78[12]
QAC_26_71	O=C([O-])C(C)C.OCC[NH2+]CCO	71[12]
QAC_27_57	O=C([O-])CCCC.OCC[NH2+]CCO	57[12]
QAC_28_37	OCC[NH+](CCO)CCO.[O-]C(=O)CCC	37[12]
QAC_29_38	OCC[NH+](CCO)CCO.[O-]C(=O)CCCC	38[12]
QAC_112_70	COCCOCCOCCOCC([O-])=O.[NH3+]CCCCCCCCCCCC	70[18]
QAC_13_4	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCCCCC[N+](C)(C)CCN(C)C	4[45]
QAC_14_6	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CC[N+](CC)(CCCCCC)CCO	6[45]
QAC_15_3	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCCC[N+](CCCCC)(CCO)CCO	3[45]
QAC_19_0	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCCCCCCC[N+](C)(CCCCCCCC)CCCCCCCC	0[13]
QAC_16_51	C[N+](C)(C)CCCC.[O-]S(C)(=O)=O	51[46,47]
QAC_17_4	C[N+](CC)(CC)CC.[O-]S(=O)(=O)OC	4[46]

QAC_18_7	C[N+](CCCC)(CCCC)CCCC.[O-]S(C)(=O)=O	7[47]
QAC_110_67	CC[NH2+]CC.[O-]C(C)=O	67[35]
QAC_111_61	CC[NH+](CC)CC.[O-]C(C)=O	61[35]
QAC_89_18	CC[N+](CC)(CC)CC.[O-]C(=O)C(N)CS	18[21]
QAC_90_19	[O-]C(=O)C(N)CS.CCCC[N+](CCCC)(CCCC)CCCC	19[21]
QAC_146_18	[O-]C(=O)[C@@H]1CCCN1.CCCC[N+](CCCC)(CCCC)CCCC	18[48]
QAC_148_24	[O-]C(=O)[C@@H]1C[C@@H](O)CN1.CCCC[N+](CCCC)(CCCC)CCCC	24[48]
QAC_5_21	[N+](CCCC)(CCCC)(CCCC)CCCC.[O-]C(=O)[C@@H]1[C@@H](O)[C@H](O)[C@@H](O)C(O)O1	21[49]
QAC_7_16	[O-]C(=O)[C@H](C)O.CCCC[N+](CCCC)(CCCC)CCCC	16[49]
QAC_8_16	[O-]C(=O)[C@@H](O)[C@H](O)C(O)=O.CCCC[N+](CCCC)(CCCC)CCCC	16[49]
QAC_9_14	[O-]C(=O)[C@@H](O)CC(=O)O.CCCC[N+](CCCC)(CCCC)CCCC	14[49]
QAC_10_1	[O-]C(=O)CCC(=O)O.CCCC[N+](CCCC)(CCCC)CCCC	1[49]
QAC_11_10	CCCC[N+](CCCC)(CCCC)CCCC.[O-]C(=O)CC(O)=O	10[49]
QAC_12_12	CC(=O)C([O-])=O.CCCC[N+](CCCC)(CCCC)CCCC	12[49]
QAC_80_83	CCCC[N+](CCCC)(CCCC)CCCC.[O-]C(=O)CCCCCCCC	83[50]
QAC_142_72	C[N+](C)(CCCC)CCCC.[O-]C(=O)C(C)O	72[51]
QAC_143_69	O=C([O-])CC(O)(CC(=O)[O-])C([O-])=O.CCCC[N+](C)(C)CCCC	69[51]
QAC_63_5	CCCCCCCCCC[N+](C)(C)CCCCCCCCCC.[O-]C(=O)CCCCCCCCCCCCCCCC	5[52]
QAC_64_87	CCCCCCCCCC[N+](C)(C)CCCCCCCCCC.[O-]C(=O)CCCCCCC\C=C\CCCCCCCC	87[52]
QAC_71_100	CCCCCCCCCCCCCCCC[N+](C)(C)C.[O-]C(=O)CCCCCCCCCCCCCCCC	100[52]
QAC_72_100	CCCCCCCCCCCCCCCC[N+](C)(C)C.[O-]C(=O)CCCCCCC\C=C\CCCCCCCC	100[52]
QAC_79_11	C=CC[N+](C)(C)CC=C.[O-]C(=O)CCCCCCCC	11[50]
QAC_82_41	CCCCCCCCCCCCCCCC[N+](C)(C)C.[O-]C(=O)CCCCCCCC	41[50]
QAC_139_77	C[N+](C)(CCCC)CCCC.[O-]C(C)=O	77[51]
QAC_140_66	C[N+](C)(CCCC)CCCC.CC(=O)CCC([O-])=O	66[51]
QAC_141_45	[O-]C(=O)C(=C)CC([O-])=O.CCCC[N+](C)(C)CCCC	45[51]
QAC_144_54	C[N+](C)(CCCC)CCCC.[O-]C(=O)\C=C\C=C\C	54[51]
QAC_145_69	C[N+](C)(CCCC)CCCC.[O-]C(=O)CCC([O-])=O	69[51]
QAC_2_0	[Br-].CC[N+](CC)(CC)CC	0[49]
QAC_3_4	[OH-].CCCC[N+](CCCC)(CCCC)CCCC	4[49]

QAC_4_4	[Br-].CCCC[N+](CCCC)(CCCC)CCCC	4[1,49]
QAC_43_70	C[N+](C)(CCCCCCCCCC)CCCCCCCCCC.[O-]N=O	70[53]
QAC_138_5	[Cl-].CCCC[N+](C)(C)CCCC	5[51]
QAC_170_16	CCCCCCCCCCCCCC[N+](C)(C)CC1=CC=CC=C1.[Cl-]	16[11]
QAC_1_3	[Br-].C[N+](C)(C)C	3[49]

Data for cholinium ILs

Table S4: Biodegradability data for cholinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Chol_31_82	OCC[N+](C)(C)C.[O-]S(C)(=O)=O	82[46,47]
Chol_32_22	COCC[N+](C)(C)C.[O-]S(C)(=O)=O	22[46]
Chol_35_52	FC(F)(C(F)(F)S([O-])(=O)=O)C(F)(F)C(F)(F)F.C[N+](C)(C)CCO	52[34]
Chol_34_25	C[N+](C)(C)CCOCC.CC(=O)CCC([O-])=O	25[33]
Chol_55_70	C[N+](C)(C)CC(=O)OCC.CC(=O)CCC([O-])=O	70[33]
Chol_60_73	[Cl-].C[N+](C)(C)CCOC(=O)C=C	73[54]
Chol_61_70	[Cl-].C[N+](C)(C)CCOC(=O)C(=C)C	70[54]
Chol_37_100	O=C([O-])CCCCCCCCCCC.C[N+](C)(C)CCO	100[55]
Chol_38_80	O=C([O-])CCCCCCCCCCCCC.C[N+](C)(C)CCO	80[55]
Chol_39_85	O=C([O-])CCCCCCCCCCCCCCC.C[N+](C)(C)CCO	85[55]
Chol_40_80	O=C([O-])CCCCCCCCCCCCCCCCC.C[N+](C)(C)CCO	80[55]
Chol_53_74	O=C([O-])CN(C)C(=O)CCCCCCCCCCC.C[N+](C)(C)CCO	74[32]
Chol_77_85	C[N+](C)(CCCCCCCCCCCC)CC(=O)O.[O-]C(=O)CCCCCCCC	85[50]
Chol_2_73	O=C([O-])C(C)N.C[N+](C)(C)CCO	73[56,57]
Chol_3_69	O=C([O-])C(N)C(C)C.C[N+](C)(C)CCO	69[56]
Chol_4_72	O=C([O-])C(N)CC(C)C.C[N+](C)(C)CCO	72[56]
Chol_5_72	O=C([O-])C(N)C(C)CC.C[N+](C)(C)CCO	72[56]
Chol_6_76	OCC(N)C([O-])=O.C[N+](C)(C)CCO	76[56,57]
Chol_7_73	OCC[N+](C)(C)C.[O-]C(=O)C(N)C(C)O	73[56,57]
Chol_8_65	[O-]C(=O)C(N)CCSC.C[N+](C)(C)CCO	65[56,57]
Chol_9_82	OC(=O)CC(N)C([O-])=O.C[N+](C)(C)CCO	82[21,56,57]

Chol_10_84	OC(=O)CCC(N)C([O-])=O.C[N+](C)(C)CCO	84[56,57]
Chol_11_86	O=C([O-])C(N)CC(N)=O.C[N+](C)(C)CCO	86[56]
Chol_12_84	O=C([O-])C(N)CCC(N)=O.C[N+](C)(C)CCO	84[56]
Chol_13_67	O=C([O-])C(N)CCCCN.C[N+](C)(C)CCO	67[56]
Chol_30_67	OCC[N+](C)(C)C.[O-]C(=O)C(N)CS	67[21]
Chol_1_74	O=C([O-])CN.C[N+](C)(C)CCO	74[21,56]
Chol_18_68	O=C([O-])C.C[N+](C)(C)CCO	68[35,56]
Chol_19_68	NC(Cc1ccccc1)C([O-])=O.C[N+](C)(C)CCO	68[21,56,57]
Chol_20_69	OCC[N+](C)(C)C.[O-]C(=O)C1CCCC1	69[28]
Chol_21_69	[O-]C(=O)CC1CCCC1.C[N+](C)(C)CCO	69[28]
Chol_22_69	[O-]C(=O)C1CCCCC1.C[N+](C)(C)CCO	69[28]
Chol_23_73	C[N+](C)(C)CCO.[O-]C(=O)CCC1CCCCC1	73[28]
Chol_24_71	[O-]C(=O)c1ccccc1.C[N+](C)(C)CCO	71[28]
Chol_25_60	O=C([O-])c1ccccc1O.C[N+](C)(C)CCO	60[28]
Chol_26_42	C[N+](C)(C)CCO.[O-]C(=O)COc1ccc2ccccc2c1	42[28]
Chol_27_49	C[N+](C)(C)CCO.[O-]C(=O)c1c2ccccc2cc2ccccc21	49[28]
Chol_33_70	CC(=O)CCC([O-])=O.C[N+](C)(C)CCO	70[33]
Chol_36_56	O=C([O-])C(F)(F)C(F)(F)C(F)(F)C(F)(F)F.C[N+](C)(C)CCO	56[34]
Chol_44_5	OCC[N+](C)(C)CC(N[C@@H](CC1=CC=CC=C1)C(O)=O)=O.[Br-]	5[26]
Chol_45_19	OCC[N+](C)(C)CC(N[C@@H](CC1=CC=CC=C1)C(OCC)=O)=O.[Br-]	19[22,23,26]
Chol_46_21	O=C([C@H](CC1=CC=CC=C1)NC(C[N+](C)(CCO)C)=O)OCCCC.[Br-]	21[23]
Chol_47_30	O=C([C@H](CC1=CC=CC=C1)NC(C[N+](C)(CCO)C)=O)OCCCCCC.[Br-]	30[23]
Chol_48_36	OCC[N+](C)(C)CC(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCCC)=O)=O.[Br-]	36[23]
Chol_49_37	OCC[N+](C)(CC(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCCCCC)=O)=O)C.[Br-]	37[23,25]
Chol_50_20	OCC[N+](C)(CC(N[C@@H](CC1=CC=CC=C1)C(OCCCCCCCCCCCCC)=O)=O)C.[Br-]	20[23]
Chol_51_20	CCOC([C@H](CC1=CC=C(O)C=C1)NC(C[N+](C)(C)CCO)=O)=O.[Br-]	20[22]
Chol_71_70	CC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	70[58]
Chol_72_46	CCCC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	46[58]
Chol_73_43	CCCCCC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	43[58]
Chol_74_44	CCCCCCCC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	44[58]
Chol_75_51	CCCCCCCCCC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	51[58]
Chol_76_60	CCCCCCCCCCCC[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	60[58]

Chol_28_78	C[N+](C)(C)CCO.[O-]C(=O)CC[C@H](C)[C@H]1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3C[C@H](O)[C@@]21C	78[28]
Chol_29_83	C[N+](C)(C)CCO.[O-]C(=O)CCC(C)C1CC[C@H]2[C@@H]3CC[C@@H]4C[C@H](O)CC[C@]4(C)[C@H]3CCC12C	83[28]
Chol_14_66	NC(Cc1cnc[NH]1)C([O-])=O.C[N+](C)(C)CCO	66[21,56,57]
Chol_15_70	O=C([O-])C(N)CCCNC(=N)N.C[N+](C)(C)CCO	70[56,57]
Chol_16_68	OCC[N+](C)(C)C.[O-]C(=O)C1CCCN1	68[21,56]
Chol_17_71	C[N+](C)(C)CCO.[O-]C(=O)C(N)Cc1c[NH]c2ccccc21	71[56,57]
Chol_52_94	C[N+](C)(C)CCO.[O-]C(=O)CCCc1c[NH]c2ccccc21	94[58]
Chol_88_81	[Br-].CC(=O)OCC1OC(OCC[N+](C)(C)C)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O	81[59]
Chol_89_57	[Br-].CC(=O)OCC1OC(OCC[N+](C)(C)CCCCCCCCCCCCC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O	57[59]
Chol_90_31	[Br-].CC(=O)OCC1OC(OCC[N+](C)(C)CCCCCCCCCCCCCCCCC)C(OC(C)=O)C(OC(C)=O)C1OC(C)=O	31[59]
Chol_67_72	Clc1cc(Cl)ccc1OCC([O-])=O.CCCCCCCCCCCCC[N+](C)(C)CC(=O)O	72[60]
Chol_68_59	Clc1cc(C)c(OCC([O-])=O)cc1.CCCCCCCCCCCCC[N+](C)(C)CC(=O)O	59[60]
Chol_69_51	Clc1cc(C)c(OC(C)C([O-])=O)cc1.CCCCCCCCCCCCC[N+](C)(C)CC(=O)O	51[60]
Chol_70_42	COc1c(c(Cl)ccc1Cl)C([O-])=O.CCCCCCCCCCCCC[N+](C)(C)CC(=O)O	42[60]
Chol_62_37	Clc1cc(C)c(OCC([O-])=O)cc1.C=CC(=O)OCC[N+](C)(C)C	37[54]
Chol_63_29	Clc1cc(C)c(OCC([O-])=O)cc1.C=C(C)C(=O)OCC[N+](C)(C)C	29[54]
Chol_64_90	COc1c(c(Cl)ccc1Cl)C([O-])=O.CC(=O)OCC[N+](C)(C)C	90[61]
Chol_65_70	Clc1cc(Cl)ccc1OCC([O-])=O.CC(=O)OCC[N+](C)(C)C	70[61]
Chol_66_80	Clc1cc(C)c(OCC([O-])=O)cc1.CC(=O)OCC[N+](C)(C)C	80[61]
Chol_56_87	Clc1cc(Cl)ccc1OCC([O-])=O.C[N+](C)(C)CC(=O)O	87[62]
Chol_57_69	Clc1cc(C)c(OCC([O-])=O)cc1.C[N+](C)(C)CC(=O)O	69[62]
Chol_58_57	Clc1cc(C)c(OC(C)C([O-])=O)cc1.C[N+](C)(C)CC(=O)O	57[62]
Chol_59_48	COc1c(c(Cl)ccc1Cl)C([O-])=O.C[N+](C)(C)CC(=O)O	48[62]
Chol_78_76	Clc1cc(Cl)ccc1OCC([O-])=O.O=C(O)CC(O)C[N+](C)(C)C	76[62]
Chol_79_59	Clc1cc(C)c(OCC([O-])=O)cc1.O=C(O)CC(O)C[N+](C)(C)C	59[62]
Chol_80_49	Clc1cc(C)c(OC(C)C([O-])=O)cc1.O=C(O)CC(O)C[N+](C)(C)C	49[62]
Chol_81_44	COc1c(c(Cl)ccc1Cl)C([O-])=O.O=C(O)CC(O)C[N+](C)(C)C	44[62]

Data for phosphonium ILs

Table S5: Biodegradability data for phosphonium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Phos_28_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC=C.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_30_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)COC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_32_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCO.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_20_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_22_2	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	2[63]
Phos_24_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_26_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCCCOC(=O)C.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	0[63]
Phos_5_7	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	7[63]
Phos_7_2	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	2[63]
Phos_9_3	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCCCC.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	3[63]
Phos_11_9	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CCCCOC(=O)C.[N-](S(=O)(=O)C(F)(F)F)S(=O)(=O)C(F)(F)F	9[63]
Phos_6_18	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCC.[O-]S(=O)(=O)OCCCCCCCC	18[63]
Phos_8_22	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCC.[O-]S(=O)(=O)OCCCCCCCC	22[63]
Phos_10_21	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCCCC.[O-]S(=O)(=O)OCCCCCCCC	21[63]
Phos_12_22	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CCCCOC(=O)C.[O-]S(=O)(=O)OCCCCCCCC	22[63]
Phos_21_15	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCC.[O-]S(=O)(=O)OCCCCCCCC	15[63]
Phos_23_20	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCC.[O-]S(=O)(=O)OCCCCCCCC	20[63]
Phos_25_30	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCCCC.[O-]S(=O)(=O)OCCCCCCCC	30[63]
Phos_27_5	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCCCOC(=O)C.[O-]S(=O)(=O)OCCCCCCCC	5[63]
Phos_29_18	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC=C.[O-]S(=O)(=O)OCCCCCCCC	18[63]
Phos_31_11	[P+](CCCCCC)(CCCCCC)(CCCCCC)COC.[O-]S(=O)(=O)OCCCCCCCC	11[63]
Phos_33_9	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCO.[O-]S(=O)(=O)OCCCCCCCC	9[63]
Phos_36_50	CCCC[P+](C)(CCCC)CCCC.COS(=O)(=O)[O-]	50[35]
Phos_1_4	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCC.[Br-]	4[63]
Phos_2_3	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCC.[Br-]	3[63]

Phos_3_2	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CC(=O)OCCCCCCCC.[Br-]	2[63]
Phos_4_9	[P+](C1CCCCC1)(C1CCCCC1)(C1CCCCC1)CCCCOC(=O)C.[I-]	9[63]
Phos_13_12	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCC.[Br-]	12[63]
Phos_14_4	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCC.[Br-]	4[63]
Phos_15_10	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC(=O)OCCCCCCCC.[Br-]	10[63]
Phos_16_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCCCOC(=O)C.[I-]	0[63]
Phos_34_9	[P+](CC)(CCCC)(CCCC)CCCC.[O-]P(=O)(OCC)OCC	9[13]
Phos_18_2	[P+](CCCCCC)(CCCCCC)(CCCCCC)COC.[Cl-]	2[63]
Phos_19_0	[P+](CCCCCC)(CCCCCC)(CCCCCC)CCO.[Br-]	0[63]
Phos_17_8	[P+](CCCCCC)(CCCCCC)(CCCCCC)CC=C.[Br-]	8[63]
Phos_38_11	CCCCCCCCCCCCCC[P+](CCCCCC)(CCCCCC)CCCCCC.C(=[N-])=NC#N	11[11]

Data for pyrrolidinium ILs

Table S6: Biodegradability data for pyrrolidinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Pyrr_21_14	[O-]S(C)(=O)=O.[O-]S(C)(=O)=O.C[N+]1(CCCC1)Cc1cn(nn1)CCOCCOCCOCCOCCOCCn1cc(nn1)C[N+]1(C)CCCC1	14[16]
Pyrr_16_4	CCCC[N+]1(C)CCCC1.[O-]S(=O)(=O)OC	4[46]
Pyrr_8_7	CCCC[N+]1(CCCC1)C.[N-](S(=O)(=O)F)S(=O)(=O)F	7[64]
Pyrr_7_0	CCC[N+]1(CCCC1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	0[64]
Pyrr_9_40	CCCC[N+]1(CCCC1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	40[65,66]
Pyrr_10_0	CCCCCC[N+]1(CCCC1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	0[64]
Pyrr_11_75	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.C[N+]1(CCCCCCC)CCCC1	75[64]
Pyrr_12_60	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.C[N+]1(CCCCCCCC)CCCC1	60[64]
Pyrr_13_20	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.C[N+]1(CCCCCCCCC)CCCC1	20[64]
Pyrr_14_78	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.C[N+]1(CCCCCCCCCC)CCCC1	78[64]
Pyrr_15_1	C[N+]1(CCCC1)CCOC.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	1[64,66]
Pyrr_18_0	C[N+]1(COCCOC)CCCC1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	0[66]
Pyrr_1_69	CCCCCCCC[N+]1(CCCC1)C.[Cl-]	69[2]
Pyrr_3_2	C[N+]1(CCCC1)CC#N.[Cl-]	2[2]

Pyrr_4_14	CCCC[N+]1(CCCC1)C.[Br-]	14[2]
Pyrr_2_67	C[N+]1(CCCC1)CCCO.[Cl-]	67[2]
Pyrr_6_6	C[N+]1(CCCC1)CCO.[I-]	6[2]
Pyrr_19_0	COCC[N+]1(C)CCCC1.F[B-](F)(F)F	0[66]
Pyrr_5_34	[Br-].O=C(OCC)C[N+]1(C)CCCC1	34[2]
Pyrr_20_72	CCCC[N+]1(C)CCCC1.CCCCCCCCCCCC(=O)N(C)CC([O-])=O	72[32]
Pyrr_17_37	SCC(N)C([O-])=O.C[N+]1(CC)CCCC1	37[21]

Data for morpholinium ILs

Table S7: Biodegradability data for morpholinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Morph_1_12	CCCC[N+]1(CCOCC1)C.[Br-]	12[67]
Morph_5_0	C[N+]1(CCOCC1)CCO.[I-]	0[2]
Morph_6_31	C[N+]1(CCOCC1)CCCO.[Cl-]	31[2]
Morph_7_0	C[N+]1(CCOCC1)CC#N.[Cl-]	0[2]
Morph_8_0	[Cl-].C[N+]1(Cc2ccccc2)CCOCC1	0[68]
Morph_9_30	CC[N+]1(CCOCC1)C.[Br-]	30[67]
Morph_10_3	CCCCCC[N+]1(CCOCC1)C.[Br-]	3[67]
Morph_11_4	[Br-].C[N+]1(CCCCCCCC)CCOCC1	4[67]
Morph_12_5	CCCCCCCCCC[N+]1(CCOCC1)C.[Br-]	5[67]
Morph_13_0	C[N+]1(CCCC)CCOCC1.FC(F)(F)C(C(F)(F)F)O[Al-](OC(C(F)(F)F)C(F)(F)F)(OC(C(F)(F)F)C(F)(F)F)OC(C(F)(F)F)C(F)(F)F	0[30]
Morph_14_17	C[N+]1(CC(N[C@@H](CC2=CC=CC=C2)C(OCC)=O)=O)CCOCC1.[Br-]	17[22]
Morph_15_100	O=C([O-])CN(C)C(=O)CCCCCCCCCCC.C1C[NH2+]CCO1	100[32]

Data for DABCO ILs

Table S8: Biodegradability data for DABCO ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
DABCO_1_0	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCCCCC[N+]12CCN(CC1)CC2	0[45]
DABCO_2_0	FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F.CCCCCCC[N+]12CCN(CC1)CC2	0[45]
DABCO_3_0	N#C[N-]C#N.OCC[N+]12CCN(CC1)CC2	0[45]
DABCO_4_40	CC[N+]12CCN(CC1)CC2.[Br-]	40[67]
DABCO_5_37	CCCC[N+]12CCN(CC1)CC2.[Br-]	37[67]
DABCO_6_22	[Br-].CCCCCC[N+]12CCN(CC1)CC2	22[67]
DABCO_7_35	CCCCCCCC[N+]12CCN(CC1)CC2.[Br-]	35[67]
DABCO_8_35	[Br-].CCCCCCCCCC[N+]12CCN(CC1)CC2	35[67]

Data for piperidinium ILs

Table S9: Biodegradability data for piperidinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Piperi_1_0	CCCC[N+]1(CCCCC1)C.[Br-]	0[2]
Piperi_2_3	CCC[N+]1(CCCCC1)C.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	3[2]
Piperi_3_79	C[N+]1(CCCCC1)CCCO.[Cl-]	79[2]
Piperi_4_29	C[N+]1(CCCCC1)CCO.[Cl-]	29[2]
Piperi_5_5	C[N+]1(CCCCC1)CC#N.[Cl-]	5[2]
Piperi_8_28	C[N+]1(CC)CCCCC1.[O-]C(=O)C(N)CS	28[21]
Piperi_9_100	O=C([O-])CN(C)C(=O)CCCCCCCCCCC.[NH2+]1CCCCC1	100[32]

Data for piperazinium ILs

Table S10: Biodegradability data for piperazinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Pipera_1_1	C[N+]1(CCCCCC)CCN(C)CC1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	1[45]
Pipera_2_1	C[N+]1(CCCCCCC)CCN(C)CC1.FC(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	1[45]

Data for prolinium ILs

Table S11: Biodegradability data for prolinium ILs.

IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Prol_1_23	O=C(C[N@+]1(C)CCC[C@@]1([H])C(OCC)=O)N[C@@H](CC2=CC=CC=C2)C(OCC)=O.[Br-]	23[22,26]
Prol_2_19	OC([C@]1([H])[N+](CC(N[C@@H](CC2=CC=CC=C2)C(OCC)=O)=O)(C)CCC1)=O.[Br-]	19[26]
Prol_3_15	CCOC([C@]1([H])[N+](CC(N[C@@H](CC2=CC=CC=C2)C(O)=O)=O)(C)CCC1)=O.[Br-]	15[26]

Data for thiazolium ILs

Table S12: Biodegradability data for thiazolium ILs.

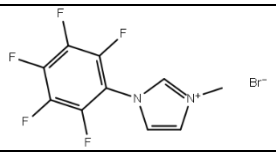
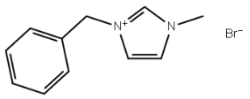
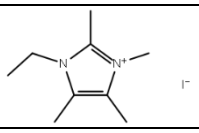
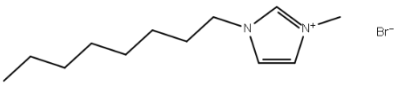
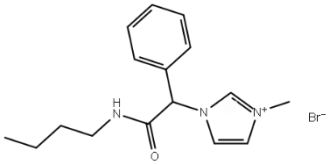
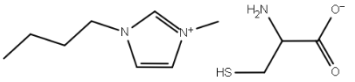
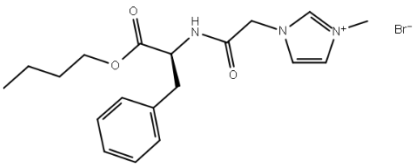
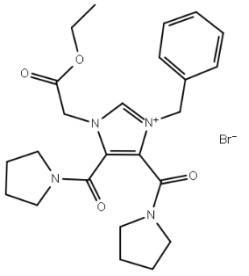
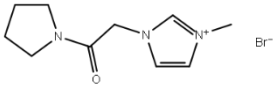
IL (cation_number_ biodegradation rate)	SMILES	biodegradation rate in %
Thia_1_3	CC[n+]1ccsc1.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	3[44]
Thia_2_7	c1csc[n+]1CCO.C(F)(F)(F)S(=O)(=O)[N-]S(=O)(=O)C(F)(F)F	7[44]

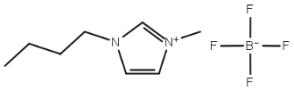
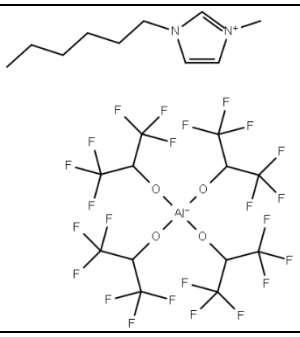
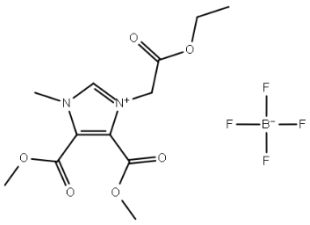
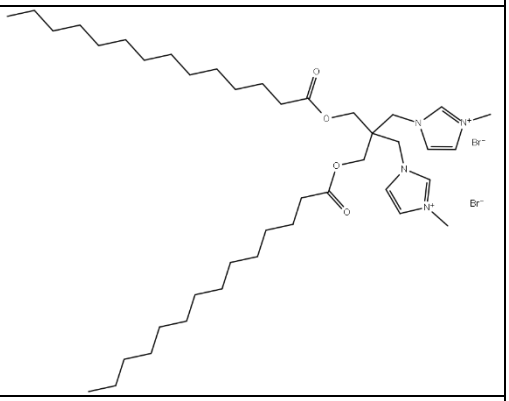
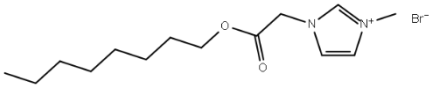
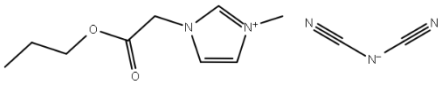
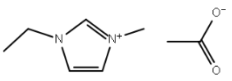
Clustering of ILs per cation core structure: Structural features of ILs

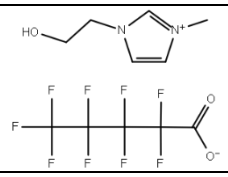
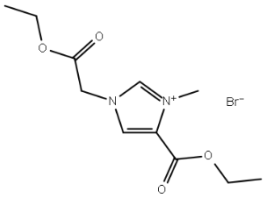
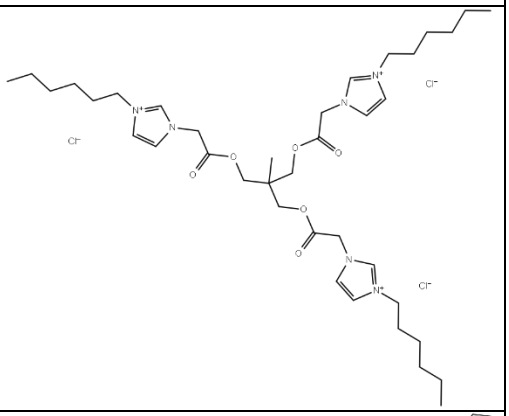
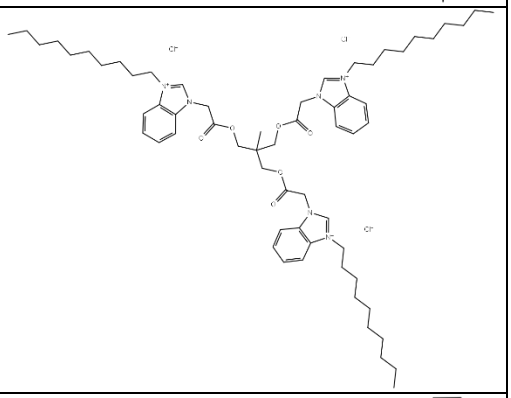
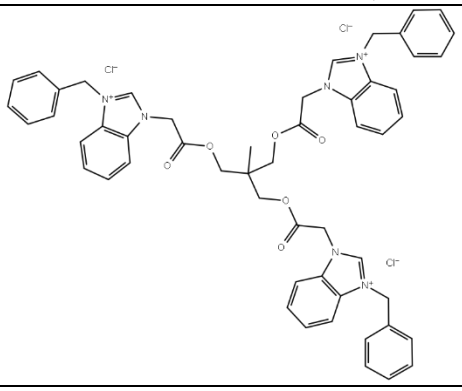
Structural features of imidazolium ILs for every cluster

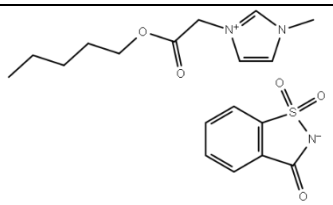
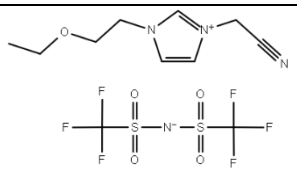
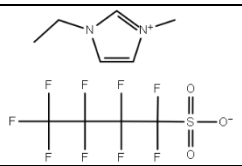
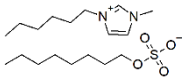
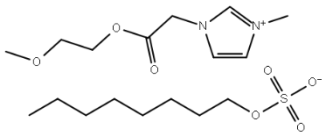
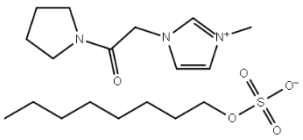
The imidazolium ILs were divided into 27 cluster thereby indicating a structurally diverse set of compounds. For every cluster a cluster centroid was generated, which represents the structural features of the ILs (Table S13). However, not every cluster centroid incorporates all structural features of the ILs within a cluster. Both ILs in cluster 1 contain at least one phenyl group, which is in one IL fully fluorinated. In cluster 2 all ILs incorporate a halogenide anion (bromide or chloride). The cation is twofold substituted with methyl and either cyano, benzyl, ethyl or ethenyl. This indicates variations in the cation. However, there was no distinct shared structural feature. The same applies for the cluster 11 and 15. The anions as well as the cations show no distinct shared structural feature. In cluster 11 the anion are tetrafluoroborate or hexafluorophosphate or tetrahexafluoroisopropoxyaluminate or dibutylphosphate. The cations contain alkyl chains and/or ester groups or ethenyl. Three out of six ILs have the tetrahexafluoroisopropoxyaluminate anion in common, two of six the fluorinated inorganic anion and a cation with ester groups. In cluster 15 the anions are dicyanamide or lauroyl sarcosinate or trifluoroacetate, while the cations incorporate only alkyl chains or cyano and ether or ester and an n-alkyl chain as functional groups. Three of five ILs have a cyano in common either in the cation or in the anion, while two ILs share the lauroyl sarcosinate anion. The cations in cluster 3 and 4 have n-alkyl side chains in common. In contrast to cluster 4, the cations in cluster 3 are fourfold or fivefold substituted by n-alkyl chains shorter than propyl. In cluster 4 the alkyl chains are longer than butyl. While in cluster 3 all anions are iodide, in cluster 4 the anions are bromide, chloride, iodide or dicyanamide. In cluster 4 some ILs are also dicationic only substituted with n-alkyl chains. This is difference to the dicationic ILs in cluster 13, which contain ester groups in side chains. The ILs in cluster 6 are characterized by amino acid anions and n-alkyl side chains attached to the cation. In cluster 7 the cation possesses amino acids in side chains and the anion is bromide. Both ILs in cluster 8 have a bromide anion and the same side chains of the cation (pyrrolidine amide, ethylacetate, benzyl side chains). The difference between them is that one IL contains two pyrrolidine amide side chains. Cluster 9 shows the amide group as structural feature of all ILs and the anions are either bromide or tetrafluoroborate. The pyrrolidine amide, as in cluster 8, is also present in most of the ILs, but in contrast to cluster 8 the ethylacetate side chain is absent. Both ILs in cluster 5 contain also the amide group in the cation, but in contrast to cluster 8 and 9, the nitrogen atom is linked only twice to carbon and additionally once to hydrogen. The ILs in cluster 10 are characterized by a fluorinated inorganic anion (tetrafluoroborate or hexafluorophosphate) and a cation substituted with two n-alkyl chains. This makes the difference to cluster 12, where the anion is also tetrafluoroborate. Cluster 12, 14 and 18 have in common a cation containing one or more ester groups. Some cations are the same in cluster 12 and 18, but they differ in the anion. In cluster 12 all ILs incorporate a tetrafluoroborate anion, while in cluster 14 and 18 the bromide or iodide anion is prevalent. The structures in cluster 14 are different to cluster 12 and 18 as they incorporate longer n-alkyl side chains (< C3). Cluster 16 is characterized by cations with alkyl side chains, while all anions contain a carboxyl group. In cluster 17 the cation is for both ILs the same (1-(2-hydroxyethyl)-3-methylimidazolium), but the anion is either perfluoropentanoate or bromide. The ILs in cluster 16 and 17 with a perfluoropentanoate anion were not allocated to the same cluster because the cations are different (only alkyl chains or hydroxyethyl, respectively). Tris and tetrakis cations are allocated to cluster 19 and 20, which only differ in the imidazolium cation (cluster 19) and benzimidazolium cation (cluster 20). For both cluster the structural features are n-alkyl chains and ester groups in the cation as well as a chloride anion. Two ILs were excluded from the cluster analysis since their molecular size was too high. Due to their structure (tetrakis benzimidazolium cation with decyl or dodecyl alkyl chains) they would have been allocated to cluster 20. Furthermore, tris and tetrakis ILs are in cluster 21, which partially also have a benzimidazolium cation, but differ from the ILs in cluster 19 and 20 as the side chains end with a benzyl group and not with a n-alkyl chain. In cluster 22 and 23 the unique structural feature of the ILs are the anions, which only appear in these clusters. In cluster 22 it is the saccharinate anion and in cluster 23 the bis(trifluoromethylsulphonyl)amide anion. The cations are more diverse and contain n-alkyl chains or ester (cluster 22 and 23) or ether or cyano (cluster 23). The ILs in cluster 24 have a sulphonate group in the anion in common, while the cations contain either only n-alkyl chains or a hydroxyl group. In cluster 25, 26 and 27 all ILs contain an alkylsulphate anion. While for cluster 27 this is the octylsulphate anion, in cluster 25 and 26 the alkyl chain in the anion varies (hexyl, heptyl, octyl, nonyl, decyl or dodecyl) and in cluster 26 there is also one IL with a methanesulphonate anion. The cationic structure of these ILs explains the distribution in these clusters. In cluster 25 all cations have n-alkyl, benzyl or ethenyl side chains, whereas in cluster 26 an ester group is the prevailing structural feature in the side chains and in cluster 27 an amide group (Table S13).

Table S13: Cluster centroids for imidazolium ILs and structural features per cluster.

No.	Structural features	Number of ILs	Cluster centroid
1	Twofold substituted cation, substituents of the first IL: fluorinated phenyl and methyl, second IL: benzyl, bromide anion	2	
2	Twofold substituted cation, first side chain is methyl and second side chain is benzyl or cyano or allyl or ethyl, bromide or chloride anion	4	
3	Four- or fivefold substituted cation, substituents: ethyl or methyl or isopropyl, iodide anion	3	
4	Twofold and fourfold substituted cation or dicationic cations; dicationic ILs: cations connected via alkyl chains (ethyl, butyl, hexyl), alkyl chain as second substituent at each cation (methyl, hexyl, dodecyl, tetradecyl, hexadecyl), bromide anion; twofold substituted cation: first side chain is methyl or ethenyl or phenyl, second side chain is butyl or hexyl or octyl or decyl or dodecyl or hexadecyl, halogenide anion (bromide, chloride, iodide), dicyanamide anion; fourfold substituted cation: first side chain is hexyl, three methyl side chains, iodide anion	19	
5	Twofold substituted cation, first side chain is methyl, second side chain contains butylcarbamoylmethyl, one IL contains an additional benzyl rest at the methyl of the butylcarbamoylmethyl group, bromide anion	2	
6	Twofold substituted cation, first side chain is methyl, ethyl or butyl or hexyl as second side chain, L-prolinate anion or L-valinate anion or L-cysteinate or L-histidinate or L-phenylalaninate or L-aspartate or glycinate anion	9	
7	Twofold substituted cation, one cation with two phenylalanine side chains, for the others first side chain is methyl, second side chain is phenylalanine group with attached alkyl chains (C2, C4, C6, C8, C10, C12) or tyrosine group with attached ethyl chain or a dipeptidyl phenylalanine-leucine chain, bromide anion	9	
8	Threefold and fourfold substituted cation; threefold substituted cation: pyrrolidine amide and ethylethanoate and benzyl side chains; fourfold substituted cation: two pyrrolidine amide side chains and ethylethanoate and benzyl side chains, bromide anion	2	
9	Twofold and threefold substituted cation; twofold substituted cation: methyl or benzyl as first side chain, pyrrolidine amide or n-butyl-N-methylcarbamoylmethyl or N,N-diethylcarbamoylmethyl as second side chain; threefold substituted cation: methyl as first	7	

	side chain, pyrrolidine amide side chain as second side chain, methyl or amide as third side, bromide anion or tetrafluoroborate anion		
10	Twofold substituted cation, first side chain is methyl, second side chain is propyl or butyl or decyl, tetrafluoroborate anion or hexafluorophosphate anion	4	
11	Twofold and threefold substituted cation; twofold substituted cation: methyl and propylethanoate or butyl or hexyl or propenyl; threefold substituted cation: two methyl side chains and butyl as third side chain, tetrahexafluoroisopropoxyaluminate or tetrafluoroborate anion, hexfluorophosphate anion or dibutylphosphate	6	
12	Twofold, threefold and fourfold substituted cation; twofold substituted cation: methyl and methylethanoate side chains; threefold substituted cation: methyl and ethylethanoate and ethylmethanoate or two methyl side chains and 2-methylpropylmethanoate; fourfold substituted cation: two methyl side chains and two methylmethanoate or methyl and two methylmethanoate and ethylethanoate or benzyl and two methylmethanoate and ethylethanoate, tetrafluoroborate anion	6	
13	Dicationic, ester group in side chain, bromide anion or chloride anion	6	
14	Twofold and threefold substituted cation; twofold substituted cation: methyl or butyl or hexyl as first side chain, propylethanoate or butylethanoate or pentylethanoate or hexylethanoate or octylethanoate or ethylbenzoate or ester of mandelic acid (C4) as second side chain; threefold substituted cation: two methyl side chains and propylethanoate or pentylethanoate, bromide anion or iodide anion	11	
15	Twofold substituted cation: methyl or acetocyano as first side chain, ethyl or butyl or propylethanoate or ethoxyethane as second side chain, dicyanamide anion or lauroyl sarcosinate or trifluoroacetate	5	
16	Twofold substituted cation: methyl as first side chain, ethyl or butyl as second side chain, lactate anion or levulinate (oxopentanoate) or acetate anion or perfluoropentanoate anion	4	

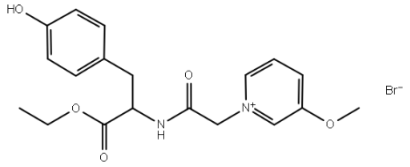
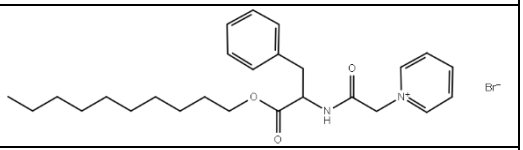
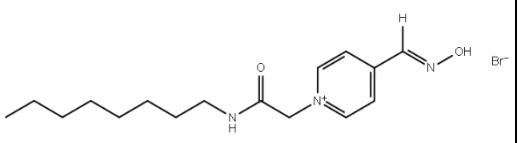
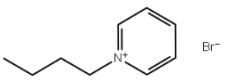
17	Twofold substituted cation: methyl as first side chain, hydroxyethyl as second side chain, perfluoropentanoate anion or bromide anion	2	
18	Twofold, threefold and fourfold substituted cation; twofold substituted cation: methyl as first side chain and ester of mandelic acid (C1, C2) or acetic acid or methylethanoate or ethylethanoate as second side chain; threefold substituted cation: methyl and ethylethanoate and ethylmethanoate side chains or two methyl side chains and 2-methylpropylmethanoate or methyl and amide and methylethanoate; fourfold substituted cation: two methyl side chains and two methylmethanoate or two methylethanoate and benzyl and ethylethanoate, bromide or iodide anion	10	
19	Tris- and tetrakis side chains: (N-butyl-imidazoliumyl-acetayloxy)methyl or (N-hexyl-imidazoliumyl-acetayloxy)methyl or (N-octyl-imidazoliumyl-acetayloxy)methyl or (N-decyl-imidazoliumyl-acetayloxy)methyl or (N-dodeyl-imidazoliumyl-acetayloxy)methyl, chloride anion	10	
20	Benzimidazolium cation, tris- and tetrakis side chains: (N-butyl-benzimidazoliumyl-acetayloxy)methyl or (N-hexyl-benzimidazoliumyl-acetayloxy)methyl or (N-octyl-benzimidazoliumyl-acetayloxy)methyl or (N-decyl-benzimidazoliumyl-acetayloxy)methyl or (N-dodecyl-benzimidazoliumyl-acetayloxy)methyl, chloride anion	8	
21	Tris- and tetrakis side chains: (N-benzyl-benzimidazoliumyl-acetayloxy)methyl or (N-benzyl-imidazoliumyl-acetayloxy)methyl, chloride anion	4	

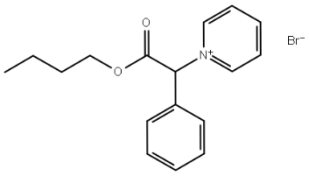
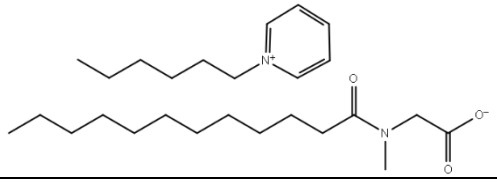
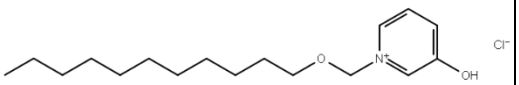
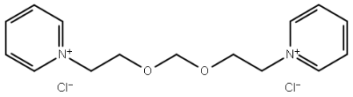
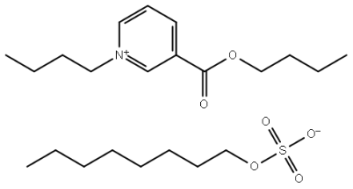
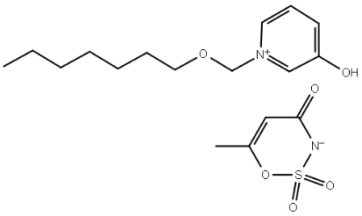
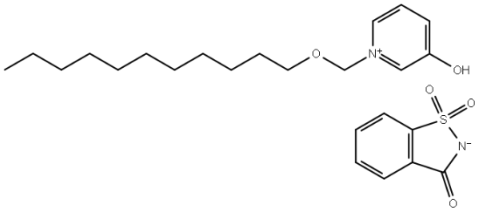
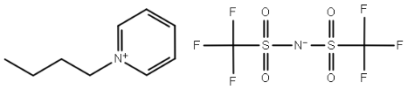
22	Twofold substituted cation: methyl as first side chain, butyl or pentylethanoate as second side chain, saccharinate anion	2	
23	Twofold substituted cation: methyl or acetocyano as first side chain, butyl or ester or ether as second side chain, bis(trifluoromethylsulphonyl)amide anion	5	
24	Twofold substituted cation: methyl as first side chain, ethyl or butyl or hydroxyethyl as second side chain, methanesulphonate anion or perfluorobutanesulphonate	3	
25	Twofold substituted cation: methyl or ethenyl as first side chain, benzyl or propenyl or butyl or hexyl as second side chain, hexylsulphate anion or heptylsulafte anion or octylsulphate anion or nonylsulphate anion or decylsulafte anion or dodecylsulphate anion	15	
26	Twofold and threefold substituted cation; twofold substituted cation: methyl as first side chain, second chain contains ester or a combinations of ester and ethers; threefold substituted cation: two methyl side chains, third side chain incorporates ester or a combinations of ester and ethers, octylsulphate anion or dodecylsulphate anion or methanesulphonate anion	18	
27	Twofold and threefold substituted cation; twofold substituted cation: methyl and acetyl pyrrolidine or N,N-bis(2-methoxyethyl)acetamide; threefold substituted cation: two methyl chains and acetyl pyrrolidine, octylsulphate anion	3	

Structural features of pyridinium ILs for every cluster

12 cluster were generated for 96 pyridinium ILs and the cluster centroids show the representative structural features of each cluster (Table S14). The ILs in cluster 1 have a bromide anion in common and an ester or carboxyl group in side chains of the cation. These could be incorporated in a phenylalanine or tyrosine moiety. Further substituents could be a methoxy group or a dimethylamino group. For the ILs in cluster 2 the structural feature of the cation is a phenylalanine moiety with different n-alkyl chains attached and a bromide anion. In cluster 3 all cations contain an amide group in the substituents, which are either acetamide, n-butyl-2-phenylacetamide or n-acetyl-L-alanine amide or 2-acetamido-3-phenylpropanamide. A further substituent could be hydroxyimino methyl in m- and p- and o-position. All anions are bromide. The ILs in cluster 4 have in common that all cations incorporate either different n-alkyl chains or benzyl or cyanomethyl, while the anions encompass bromide, chloride, hexafluorophosphate and dicyanamide. The ILs in cluster 5 possess different structural features, which cannot be combined under a general category. All have in common an ester in the cation or a carboxyl group in the anion. The ILs with an ester in the cation incorporate inorganic anions, like bromide, iodide and hexafluorophosphate. The cations contain either ethyl methanoate or ethyl ethanoate or butyl methanoate or ester derived from mandelic acid. Further substituents could be benzyl, alkyl chains, methoxy. The IL without an ester in the cation shows a carboxyl group in the perfluoropentanoate anion, while the cation is substituted by n-alkyl chains. In cluster 6 all ILs contain a lauroyl sarcosinate anion and the cations are substituted with n-alkyl chains. Cluster 7, 10 and 11 have the cations in common, but vary in the anion. While in cluster 7 pyridinium cations incorporate a hydroxyl group in m-position and ether groups in different alkyl chains as well as a chloride anion, in cluster 10 and 11 the cations have the same structural features and the anions are acesulfamate and saccharinate, respectively. Cluster 8 encompass single cationic and dicationic ILs incorporating an inorganic anion, like chloride, iodide, hexafluorophosphate. The single cationic ILs contain a hydroxyethyl group, while in the dicationic ILs both cations are connected via ether bonds. All pyridinium ILs with a octlysulphate anion or bis(trifluoromethylsulphonyl)amide anion are allocated to cluster 9 and 12, respectively. The cations in cluster 9 and 12 possess different structural features, which cannot be combined under a general category. The cations in cluster 9 are substituted by different n-alkyl chains or ester or ether or butylcarbamoyl. The cations in cluster 12 encompass a dicationic IL with ether bonds connecting both cations and for single cationic ILs substituents are acetic acid, allyl, benzyl, carbamate, ether, ester, hydroxyethyl and tertiary amine (Table S14).

Table S14: Cluster centroids for pyridinium ILs and structural features per cluster.

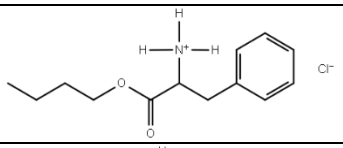
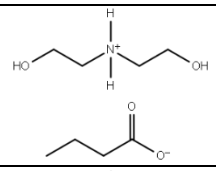
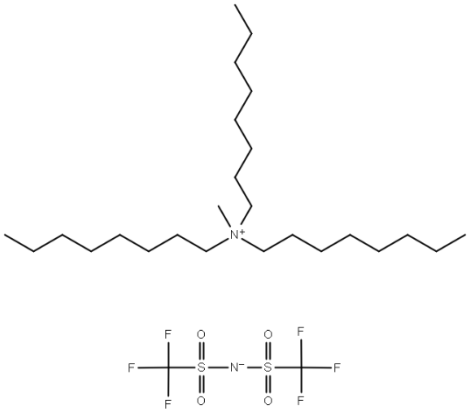
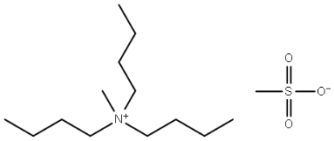
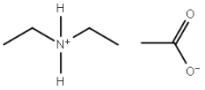
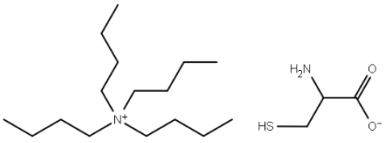
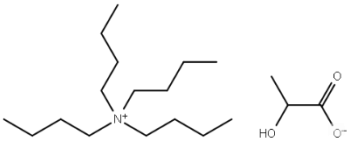
No.	Structural features	Number of ILs	Cluster centroid
1	Single or twofold substituted cation, substituents at N: acetic acid or phenylalanine group with or without attached ethyl chain or tyrosine group with attached ethyl chain, substituents in m- and p-position to substituents at N: methoxy group or dimethylamino group or acetic acid or ethyl methanoate, bromide anion	12	
2	Single substituted cation at N: acetic acid or phenylalanine group with attached alkyl chains via ester bonds (C4, C6, C8, C10, C12), bromide anion	5	
3	Single and twofold substituted cations, single substituted cation: substituents at N: n-butyl-2-phenylacetamide, twofold substituted: substituents at N: octyl chain connected to cation via acetamide or n-acetyl-L-alanine amide or 2-acetamido-3-phenylpropanamide substituents in m- and p- and o-position to substituents at N: hydroxyimino methyl bromide anion	6	
4	Single substituted cation: substituents at N: alkyl chain (C3, C4, C10, C16), benzyl, cyanomethyl, twofold substituted cation: substituents at N: alkyl chain (C4, C6, C8), substituents in m- and p-position to substituents at N: methyl, inorganic anions (bromide, chloride, hexafluorophosphate), one organic anion (dicyanamide)	13	

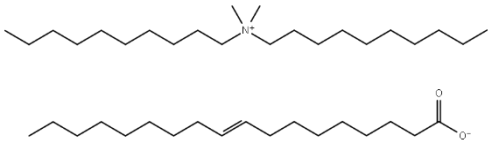
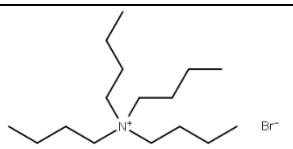
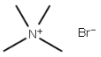
5	Single substituted cation: substituents at N: esters of mandelic acid (C1, C2, C4) or ethyl ethanoate, twofold substituted cation: substituents at N: ethyl or methyl or benzyl or esters of mandelic acid (C2, C4) or ethyl methanoate, substituents in m-position to substituents at N: methyl or methoxy or ethylmethanoate or butyl methanoate or inorganic anion (bromide, iodide, hexafluorophosphate) and one organic anion perfluoropentanoate	11	
6	Single and threefold substituted cations, single substituted cation: n-butyl or n-hexyl at N, threefold substituted cation: substituents at N: n-octyl, methyl group in m- and p-position to substituents at N, lauroyl sarcosinate anion	3	
7	twofold substituted cation, substituents at N: ether bonds in alkyl chains (propoxymethyl, heptyloxymethyl, undecyloxymethyl, octadecyloxymethyl) substituents in m-position to substituents at N: hydroxyl group, chloride anion	4	
8	Single and dicationic, single substituted cation at N: hydroxyethyl group (single cationic) or cations connected via ether bonds, (dicationic), inorganic anions (chloride, iodide, hexafluorophosphate)	4	
9	Single and twofold substituted cations, single substituted at N: butyl or ethyl ethanoate, twofold substituted: substituents at N: methyl or butyl or octyl or ethyl ethanoate or pentyl ethanoate, substituents in m-position to substituents at N: butyl methanoate or methyl or methoxymethyl or ethoxymethyl, butylcarbamoyl, octylsulphate anion	11	
10	Twofold substituted cation, substituents at N: ether bonds in alkyl chains (propoxymethyl, butoxymethyl, hexyloxymethyl, heptyloxymethyl, undecyloxymethyl, octadecyloxymethyl) substituents in m-position to substituents at N: hydroxyl group, acesulfamate anion	6	
11	Twofold substituted cation, substituents at N: ether bonds in alkyl chains (propoxymethyl, butoxymethyl, hexyloxymethyl, heptyloxymethyl, undecyloxymethyl, octadecyloxymethyl) substituents in m-position to substituents at N: hydroxyl group, saccharinate anion	6	
12	Single and dicationic, single and twofold substituted, dicationic: single substituted cations connected via ether bonds, single cationic and single substituted at N: hydroxyethyl or carbamate or butyl or ethyl ethanoate or allyl or benzyl or tertiary amine single cationic and twofold substituted: substituents at N: hydroxyethyl or ethoxymethyl or methyl or butyl, substituents in m-position to substituents at N: butyl methanoate or butyl or methoxymethyl or tertiary amine or methyl or acetic acid, bis(trifluoromethylsulphonyl)amide anion	15	

Structural features of QACs for every cluster

The 60 QACs are divided in 10 cluster (Table S15). Cluster 1 differ to the other cluster as the ILs have all a cation with a phenylalanine moiety bonded to different n-alkyl chains via an ester. The anion is chloride. Cluster 2, 5, 7 and 8 contain all ILs with anions based on carboxylic acids. In contrast to cluster 5, 7 and 8, in cluster 2, except one IL, the cations contain at least one hydroxyethyl group. In cluster 5 the ILs also incorporate acetate as anion as in cluster 2, whereas the cation is twofold or threefold substituted with linear ethyl chains. The main difference between cluster 5, 7 and 8 is that in cluster 5 the cations are twofold and threefold substituted with alkyl chains, whereas in cluster 7 and 8 the cations incorporate four alkyl side chains of different n-alkyl length. All QACs with a bis(trifluoromethylsulphonyl)amide anion are allocated to cluster 3 and all with a methylsulphonate or methylsulphate anion to cluster 4. The cations in both clusters are characterized by linear alkyl chains, while in cluster 3 some cations also contain hydroxyethyl groups or a N-(2-(dimethylamino)ethyl group. The anions in cluster 6 are all based on amino acids, while the cation is substituted by only ethyl or butyl chains. In cluster 9 the ILs contain an inorganic anion (halogenide or hydroxyl or nitrite anion), while the cation is substituted by mainly n-alkyl chains of different length. One cation also contains a benzyl group. The IL in cluster 10 also contains a halogenide anion compared to cluster 9, but only methyl chains in the cation.

Table S15: Cluster centroids for QACs and structural features per cluster.

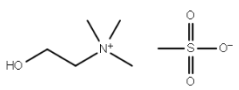
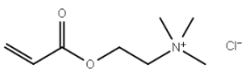
No.	Structural features	Number of ILs	Cluster centroid
1	Phenylalanine cation bonded to alkyl chains (C2, C4, C6, C8, C10, C12, C14, C16) via an ester, chloride anion	8	
2	Nitrogen in cation substituted with one or two or three hydroxyethyl chains or with one dodecyl chain, formate or acetate or propionate or butaneoate or isobutanoate or pentanoate or 2,5,8,11-tetraoxatridecan- 13-oate	11	
3	Threefold substituted cation by octyl chains and one methyl chain or twofold substituted by methyl chains and one hexyl chain and one N-(2-(dimethylamino)ethyl chain or twofold substituted by ethyl chains and one hexyl chain and one hydroxyethyl chains or twofold substituted by hydroxyl ethyl chains and one butyl chain and one pentyl chain, bis(trifluoromethylsulphonyl)amide anion	4	
4	Threefold substituted cation by methyl chains and one butyl chain or threefold substituted cation by ethyl chains and one methyl chain or threefold substituted cation by butyl chains and one methyl chain, methylsulphonate or methylsulphate	3	
5	Twofold and threefold substituted cation by ethyl side chains, acetate anion	2	
6	Fourfold substituted cation by ethyl chains or butyl chains, L-cysteinate anion or prolinate or 4-hydroxyprolinate anion	4	
7	Fourfold substituted cation by two methyl and two butyl chains or four butyl chains, L-tartrate or L-lactate or L-malate or citrate or glucoronate or succinate or malonate or pyruvate or pelargonate anion	10	

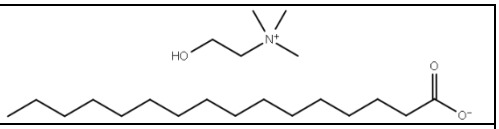
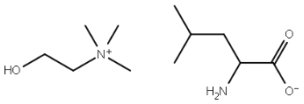
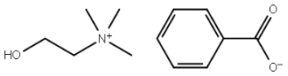
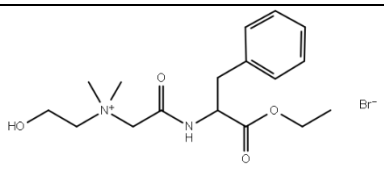
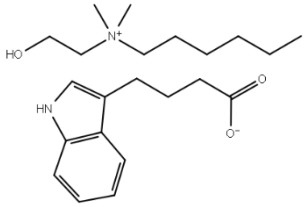
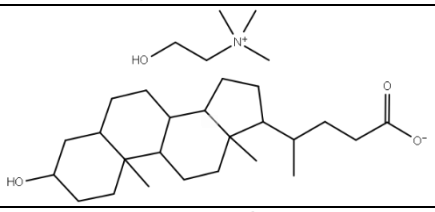
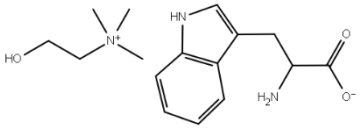
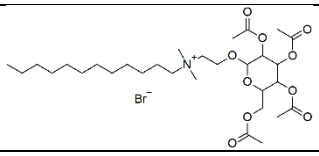
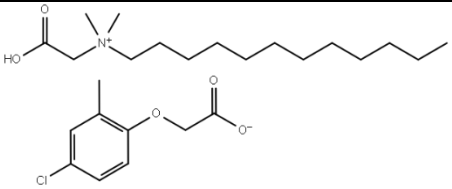
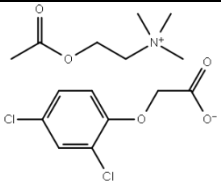
8	Fourfold substituted cation by two methyl chains and two decyl chains or three methyl chains and one hexadecyl chain or two methyl chains and two ethenyl groups or two methyl chains and two butyl chains, acetate or sorbate or succinate or levulinate or itaconate or pelargonate or stearate or oleate anion	11	
9	Fourfold substituted cation by ethyl chains or butyl chains or twofold substituted cation by methyl chains and two butyl chains or two decyl chains or tetradecyl chain and benzyl, bromide anion or chloride anion, hydroxyl anion or nitrite anion	6	
10	Fourfold substituted cation by methyl side chains, bromide anion	1	

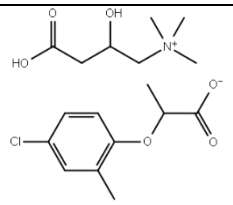
Structural features of cholinium ILs for every cluster

For analysing the biodegradation of cholinium ILs 80 compounds were grouped in 13 clusters (Table S16). The characterization of each cluster is summarized with regard to structural features of the ILs, the number of ILs per cluster and the cluster centroid (Table S16). Cluster 1 is characterized by a sulphonate anion, which is either perfluorobutanesulphonate or methylsulphonate, while the cation is cholinium. One of the three ILs contains a choline methyl ether cation and a methylsulphonate anion. The ILs in cluster 2 contain a cholinium derivative as cation. Instead of the of hydroxyethyl side chain, they incorporate diethyl ether or ethylethanoate or ethylprop-2-enoate or ethyl-2-methylprop-2-enoate. The anions are either 4-oxopentanoate or chloride. The ILs in cluster 3 contain the cholinium cation, except for one IL it is the dodecylbetainium cation. The anions are either lauroyl sarcosinate or nonanoate or dodecanoate or tetradecanoate or hexadecanoate or octadeconate anion showing all a carboxyl group and alkyl chains equal or longer than nonyl. The ILs in cluster 4 contain all the cholinium cation. The anions are all based on amino acids. Like in cluster 4, the ILs in cluster 5 contain all the cholinium cation, but vary in the anion. All anions incorporate a carboxyl group and are based on amino acids or aromatics or cycloalkyl compounds or linear alkyl carboxylic acids or keto acids. The reason why the two ILs with an amino acid anion in cluster 5 were not assigned to cluster 4 could be that the phenylalanine anion is based on an aromatic amino acid and therefore is structurally more related to the other aromatic anions in cluster 5. The glycinate anion in cluster 5 was not assigned to cluster 4 possibly because it is based on the simplest amino acid and more structurally related to the acetate anion due to the number of carbon atoms. In cluster 6 all cations incorporate a phenylalanine or a structurally related tyrosine moiety, which are bonded via an ester to an alkyl chain of varying length. The anion is bromide. The unique structural feature in cluster 7 is the indole-3-butyrate anion, while the cation is characterized by an elongated linear alkyl side chain (C2-C12), which replaces one methyl chain in the cholinium cation. In cluster 9 there is also one IL with an indole-3-butyrate anion, but the cation is the pure cholinium cation, why this IL has more structural features with the ILs in cluster 9 in common. These ILs have all the cholinium cation, while the anion is based on an amino acid. Especially the tryptophanate anion is structurally related to the indole-3-butyrate anion. The amino acid anions in cluster 9 differentiate from the ones in cluster 4 and 5 as the histidinate, prolinate and tryptophanate anion contain all a ring of five atoms, of which one is at least nitrogen, and the arginate anion is structurally not well related to the ones in cluster 4 due to its guanidine moiety. In cluster 8 the structural features of both ILs are a cholinium cation and either a desoxycholate or litocholate anion differentiating them from all other cholinium ILs. Cluster 10 contains cholinium derivatives. The cation is characterized by a D-glucose moiety in a side chain and a second side chain of different linear alkyl chains. The anion is bromide. The cluster 11, 12 and 13 have in common that the anions are based on herbicides. The cations differ as in cluster 11 the prevalent cation is dodecylbetainium, in cluster 12 the cation is an ester derivative of cholinium and in cluster 13 the cations are either betaine or carnitine (Table S16).

Table S16: Cluster centroids for cholinium ILs and structural features per cluster.

No.	Structural features	Number of ILs	Cluster centroid
1	Cholinium cation or choline methyl ether, perfluorobutanesulphonate anion or methylsulphonate anion	3	
2	Cholinium derivatives: instead of hydroxyethyl side chain: diethyl ether or ethylethanoate or ethylprop-2-enoate or ethyl-2-methylprop-2-enoate, 4-oxopentanoate anion or chloride anion	4	

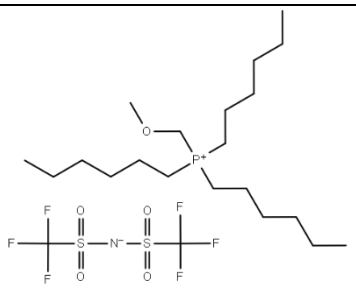
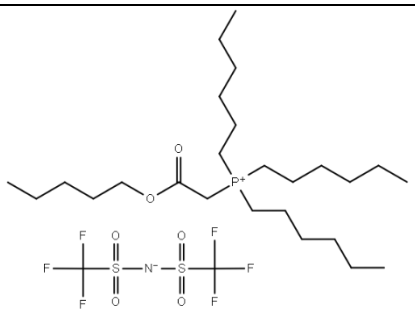
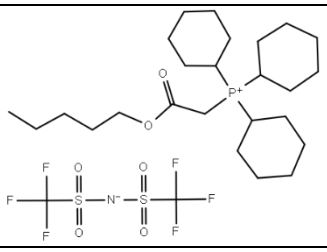
3	Cholinium cation or dodecylbetainium, lauroyl sarcosinate or nonanoate or dodecanoate or tetradecanoate or hexadecanoate or octadeconate anion	6	
4	Cholinium cation, L-alaninate or L-valinate or L-leucinate or L-isoleucinate or L-serinate or L-threoninate or L-methioniate or L-aspartate or L-glutamate or L-asparaginate or L-glutaminate or L-lysinate or L-cysteinate anion	13	
5	Cholinium cation, acetate or glycinate or phenylalaninate or 4-oxopentanoate or perfluoropentanoate or cycloalkyl anions with carboxylate group (cyclopentane carboxylate or cyclopentane acetate or cyclohexane carboxylate or cyclohexane propionate) or aromatic anions with carboxylate group (benzoate or salicylate or 2-naphthoxyacetate or anthracene-9-carboxylate)	13	
6	Cholinium derivatives: instead of one methyl side chain: phenylalanine group with attached alkyl chains via ester bonds (C4, C6, C8, C10, C12) or tyrosine group with attached alkyl chains via ester bonds (C2), bromide anion	8	
7	Cholinium derivatives: one methyl chain is changed to: ethyl or butyl or hexyl or octyl or decyl or dodecyl side chain, indole-3-butyrate anion	6	
8	Cholinium cation, salts of bile acids as anion (desoxycholate or litocholate)	2	
9	Cholinium cation, L-histidinate or L-argininate or L-prolinate or L-tryptophanate or indole-3-butyrate anion	5	
10	Cholinium derivatives: methyl or dodecyl or hexadecyl chain at positively charged N, N-[2-(2,3,4,6-tetra-O-acetyl-ß-D-glucopyranosyloxy)-ethyl]-moiety, bromide anion	3	
11	Cholinium derivatives: dodecylbetainium cation, (2,4-dichlorophenoxy)acetate or (4-chloro-2-methylphenoxy)acetate or 3,6-dichloro-2-methoxybenzoate anion or 2-(4-chloro-2-methylphenoxy)propionate	4	
12	Cholinium derivatives: acetylcholine or instead of hydroxyethyl side chain: ethylprop-2-enoate or ethyl-2-methylprop-2-enoate, (2,4-dichlorophenoxy)acetate or (4-chloro-2-methylphenoxy)acetate or 3,6-dichloro-2-methoxybenzoate	5	

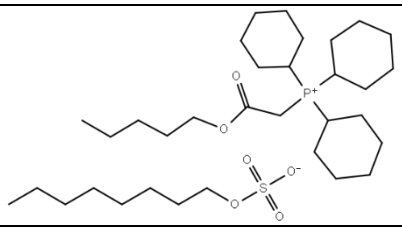
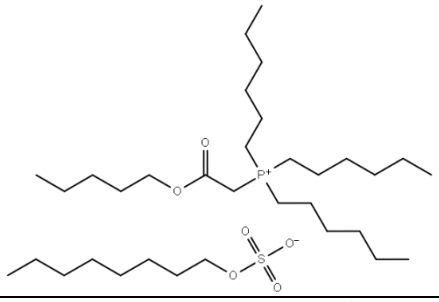
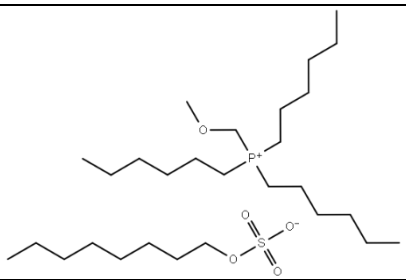
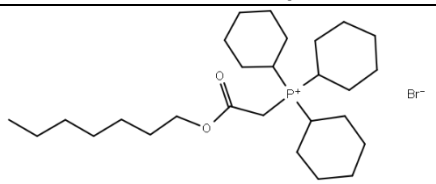
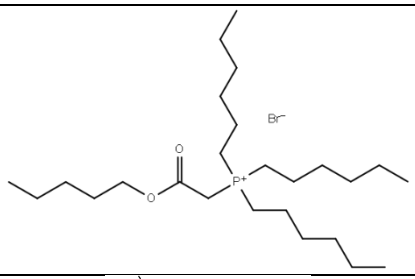
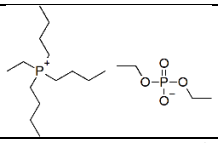
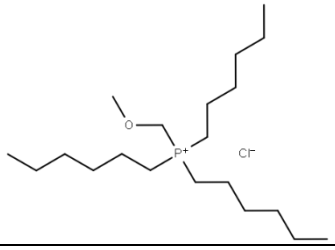
13	Cholinium derivatives: betaine or carnitine, (2,4-dichlorophenoxy)acetate or (4-chloro-2-methylphenoxy)acetate or 3,6-dichloro-2-methoxybenzoate or 2-(4-chloro-2-methylphenoxy)propionate	8	

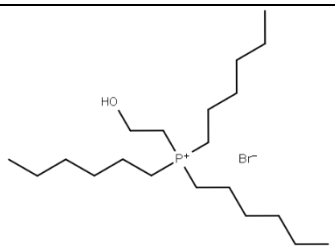
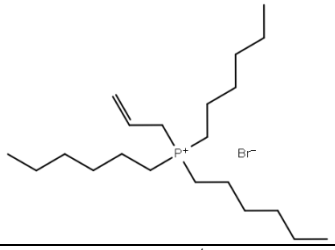
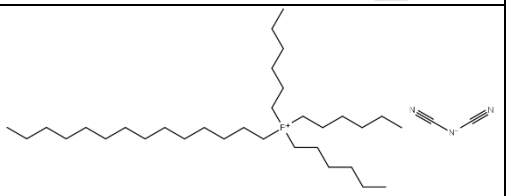
Structural features of phosphonium ILs for every cluster

The 36 phosphonium ILs have been divided into 12 clusters (Table S17). The ILs in cluster 2, 5 and 8 consist of a tri-n-hexylphosphonium cation incorporating an ester group in the fourth side chain, which underlies variations in chain length, while the anion varies too per cluster. The anions per cluster are bis(trifluoromethylsulphonyl)amide, octylsulphate and halogenide, respectively. The same applies for cluster 3, 4 and 7. In cluster 3, 4 and 7 the cation is a tri-cyclohexylphosphonium with an ester group in the fourth side chain varying in chain length, while the anions are bis(trifluoromethylsulphonyl)amide, octylsulphate and bromide or iodide, respectively. Cluster 1 and 6 have both the tri-n-hexylphosphonium cation with variations in functional groups in the fourth side chain (allyl or hydroxyl or ether) in common, but differentiate in the anion as in cluster 1 the ILs contain a bis(trifluoromethylsulphonyl)amide anion and in cluster 6 octylsulphate. In addition, the fourth IL in cluster 6 incorporates a tri-n-hexylphosphonium cation as well and a methyl group as fourth side chain. The anion is methylsulphate, which is structurally related to the octylsulphate anion of the three other ILs. The IL in cluster 9 incorporates a diethylphosphate anion and an ethyltributylphosphonium cation. The cations in cluster 10, 11 and 12 are similar to the ones in cluster 1 and 6, but the anion is a halogenide. The ILs in cluster 10, 11 and 12 are not together in one cluster because of the manual adjustments in dividing the sILs into more cluster and automatically generated cluster 10, 11 and 12, which was necessary to generate cluster 2 and 3 and to differentiate between these ILs. Cluster 13 contains the only IL with a dicyanamide anion (Table S17).

Table S17: Cluster centroids for phosphonium ILs and structural features per cluster.

No.	Structural features	Number of ILs	Cluster centroid
1	Tri-n-hexyl, fourth chain consists of either allyl or hydroxyethyl or methoxymethyl groups, bis(trifluoromethylsulphonyl)amide anion	3	
2	Tri-n-hexyl, ester group in fourth chain (propylethanoate or pentylethanoate or heptylethanoate or acetoxybutyl), bis(trifluoromethylsulphonyl)amide anion	4	
3	Tri-cyclohexyl, ester group in fourth chain (propylethanoateor pentylethanoate or acetoxybutyl or heptylethanoate), bis(trifluoromethylsulphonyl)amide anion	4	

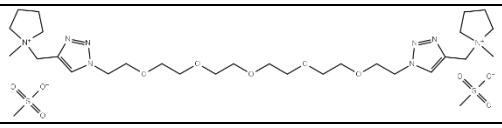
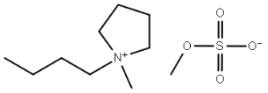
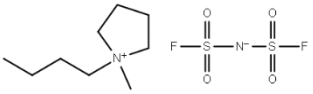
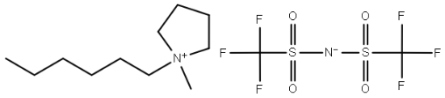
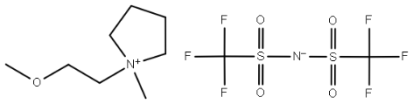
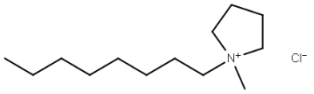
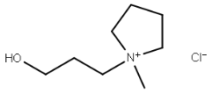
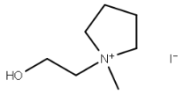
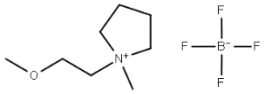
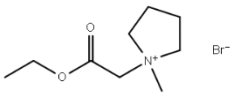
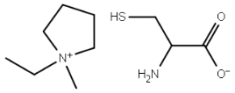
4	Tri cyclohexyl, ester group in fourth chain (propylethanoate or pentylethanoate or heptylethanoate or acetoxybutyl), octylsulphate anion	4	
5	Tri-n-hexyl, ester group in fourth chain (propylethanoate or pentylethanoate or heptylethanoate or acetoxybutyl), octylsulphate anion	4	
6	Three ILs: tri-n-hexyl, fourth chain consists of either allyl or methoxymethyl or hydroxyethyl, octylsulphate anion, fourth IL: tri-butyl, fourth chain is methyl, methylsulphate anion	4	
7	Tri-cyclohexyl, ester group in fourth chain (propylethanoate or pentylethanoate or heptylethanoate or acetoxybutyl)), halogenide anion	4	
8	Tri-n-hexyl, ester group in fourth chain (propylethanoate or pentylethanoate or heptylethanoate or acetoxybutyl, halogenide anion	4	
9	Tri-n-butyl and ethyl chains, diethylphosphate anion	1	
10	Tri-n-hexyl, methoxymethyl, chloride anion	1	

11	Tri-n-hexyl, hydroxyethyl, bromide anion	1	
12	Tri-n-hexyl, allyl group, bromide anion	1	
13	Tri-n-hexyl, tetradecyl, dicyanamide anion	1	

Structural features of pyrrolidinium ILs for every cluster

21 pyrrolidinium ILs have been divided in 11 cluster according to their similarity and are structurally characterized by a cluster centroid (Table S18). The number of clusters was adjusted manually in order to differentiate between the ILs into more detail. Cluster 1 contains the only dicationic pyrrolidinium IL. In cluster 2, 3 and 11 the cations incorporate alkyl chains, while the anions are methylsulphate, bis(fluorosulphonyl)amide and cysteinate, respectively. Cluster 4 is characterized by cations incorporating different alkyl side chains and a bis(trifluoromethylsulphonyl)amide anion. In cluster 5 and 9 ether groups are attached to the cations, while the anions are bis(trifluoromethylsulphonyl)amide and tetrafluoroborate, respectively. Cluster 6 consists of three ILs, of which two incorporate a pyrrolidinium cation with different alkyl side chains and the third IL contains an additional cyano group in the side chain, which do not show similarity at first sight. However, it was not possible to divide cluster 6 without splitting the other cluster into more cluster, which would result in a loss of generalization. Both ILs in cluster 7 and 8 contain a cation with a hydroxyl group, but differentiate in the halogenide anion. In cluster 10 both ILs are characterized by the structural feature NCCOO(H or R) either in the cation as ester or in the lauroyl sarcosinate anion as carboxyl group (Table S18).

Table S18: Cluster centroids for pyrrolidinium ILs and structural features per cluster.

No.	Structural features	Number of ILs	Cluster centroid
1	Dicationic, connected via triazole and ether bonds, methanesulphonate anion	1	
2	Butyl and methyl side chains of the cation, methylsulphate anion	1	
3	Butyl and methyl side chains of the cation, bis(fluorosulphonyl)amide anion	1	
4	Different alkyl side chains of the cation (C3, C4, C6, C7, C8, C9, C10), bis(trifluoromethylsulphonyl)amide anion	7	
5	Ether bonds in propyl, butyl side chains of the cation, bis(trifluoromethylsulphonyl)amide anion	2	
6	Different side chains of the cation (C4, C8), one IL with ethyl side chain and an additional cyano group, halogenide anion	3	
7	Propyl side chain with a hydroxyl group, chloride anion	1	
8	Ethyl side chain with a hydroxyl group, iodide anion	1	
9	Ether bond in propyl side chain of the cation, tetrafluoroborate anion	1	
10	First IL: ester bond in side chain of the cation, bromide anion; second IL: butyl, methyl side chains, carboxyl group in the anion (lauroyl sarcosinate)	2	
11	Ethyl and methyl side chains of the cation, cysteinate anion	1	

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