Supporting Information. Table S1. Cations with experimental and calculated melting points for the respective bromides ordered according to experimental melting points.

	Cation		mp(°C)	
No.	N-substituent	Other substituents	exp.	calc.
1	decyl	3-pentyl	30.0	28.0
2	11-propionyloxyundecyl		35.0	31.6
3	benzyl	4-dibenzyl; 3-ethoxycarbonyl	35.0	41.8
4	octyl	4-propyl	37.0	38.9
5	tetradecyl	4-hexyl	37.0	26.7
6	tetradecyl	3-pentyl	39.0	23.6
7	decyl	4-ethoxycarbonyl	40.5	40.4
8	dodecyl	4-propyl	41.0	32.1
9	undecyl		41.9	52.2
10	octyl	4-ethyl	42.5	39.0
11	dodecyl	4-ethyl	43.5	37.3
12	decyl		44.5	56.3
13	dodecyl		45.0	47.3
14	hexyl	2-(2-methyloctyl)	47.0	22.0
15	ethoxycarbonylmethyl	5-butyl; 2-methyl	51.0	48.8
16	2,5-dimethoxyphenethyl		53.8	59.1
17	tridecyl		54.5	48.1
18	4-fluoro-benzyl		57.5	96.4
19	tetradecyl		59.0	48.2
20	butyl	4-ethoxycarbonyl	60.0	72.7
21	2-methylpropyl		64.0	85.4
22	methyl	3-(3-hydroxypropyl)	64.0	88.6
23	benzyl	3-methyl	64.5	84.0
24	butyl	2-benzylsulfanyl	65.0	80.8
25	2-cyclohexyl-2-oxo-ethyl		69.0	86.0

No.	Cation		mp(°C)	
	N-substituent	Other substituents	exp.	calc.
26	methylpropyl		69.5	101.2
27	2-pyridinyl		70.4	103.3
28	2-(ethoxycarbonyl)ethyl		71.0	99.5
29	1-(ethoxycarbonyl)propyl		73.0	89.4
30	propyl		75.5	106.5
31	ethyl[1]	3-diethylcarbamoyl	77.0	130.1
32	2-phenoxyethyl		78.0	84.2
33	methyl	2,4,6-tetramethyl	78.5	123.5
34	methyl	4-(3-hydroxypropyl)	79.0	93.7
35	ethyl	2,6-dimethyl	80.0	107.6
36	methyl	3-pyridinyl	80.0	100.3
37	isopropyloxycarbonylmethyl		80.0	114.3
38	morpholinomethyl	4-methyl	82.5	92.4
39	methyl	4-benzyl	85.5	62.1
40	2-fluoroethyl	3-ethoxycarbonyl	87.0	115.7
41	phenethyl	4-methyl	89.9	66.9
42	butyl	3-carboxy	91.0	102.7
43	allyl	3-diethylcarbamoyl	92.0	113.5
44	bis(ethoxycarbonyl)methyl		93.5	107.7
45	4-acetoxybutyl	3-hydroxy	95.0	92.0
46	benzyloxy		95.0	86.0
47	allyl[1]		95.5	142.8
48	methyl	3-ethoxycarbonyl	96.0	128.5
49	2-hydroxyethyl	3-methyl	97.0	107.4
50	ethyl	2-methyl	97.0	121.5
51	isopropyl		97.0	98.0
52	butyl		97.5	89.4

	Cation		mp(°C)	
No.	N-substituent	Other substituents	exp.	calc.
53	ethyl	4-(4-pyridyl)	98.0	116.2
54	allyl	3-hydroxy	98.0	99.0
55	benzyl		99.0	85.0
56	methyl	4-(2-ethoxycarbonylethyl)	99.5	90.5
57	ethyl	3-acetyl	100.0	114.6
58	allyl	3-formyl	100.0	128.1
59	acetonyl[1]	2,6-dimethyl	104.0	149.5
60	ethyl	3-hydroxy	106.0	131.5
61	ethoxy	4-methoxy	108.5	143.0
62	propyloxycarbonylmethyl		110.0	115.9
63	allyl	2-hydroxymethyl	110.0	118.2
64	2-hydroxyethyl		110.0	106.8
65	allyl	4-hydroxymethyl	111.0	113.9
66	5-hexynyl		114.0	85.4
67	2-cyanoethyl	3-methyl	116.0	125.9
68	pyridinyl		118.0	100.75
69	isopropyl	4-hydroxymethyl	119.0	110.1
70	3-chloropropyl		120.0	124.3
71	ethyl		120.5	123.1
72	allyl	4-cyan	121.0	136.8
73	ethyl	4-methyl	121.0	160.1
74	isopropyl	2-hydroxymethyl	122.0	116.3
75	2-hydroxyethyl	3-hydroxy	122.5	113.6
76	2-hydroxyethyl	3,4-dimethyl	126.5	104.9
77	3,3-dimethylallyl	4-methyl	127.5	110.7
78	1-methyl-2-oxopropyl	2-methyl	133.0	132.8
79	2-cyano-ethyl	3,4-dimethyl	133.0	129.5

	Cation		mp(°C)	
No.	N-substituent	Other substituents	exp.	calc.
80	ethoxycarbonylmethyl		137.0	128.1
81	3-bromopropyl	4-methyl	139.5	106.7
82	(Z)-3-methylpent-2-en-4-inyl		139.5	115.2
83	methyl	3-methoxycarbonyl	141.0	147.4
84	2-cyanoethyl	3-amino	142.0	159.4
85	1-methyl-2-oxopropyl		144.0	125.2
86	cyanomethyl	3,5-dimethyl	144.0	144.4
87	methyl	4-methyl-3-hydroxy	145.8	148.2
88	2-cyanoethyl	4-methyl	147.0	151.4
89	2-cyanoethyl		149.0	151.3
90	methyl		150.0	142.4
91	methyl	3-hydroxy	153.5	149.9
92	vinyl		154.5	139.6
93	phenyl[1,2]		155.0	87.8
94	(E)-3-hydroxyprop-1-en-1-yl		156.5	138.8
95	2-carboxyallyl		156.5	139.3
96	cyclohex-2-enyl[1,2]		159.5	79.2
97	2-cyanoethyl[1]	3,5-dimethyl	160.5	115.9
98	3-carboxypropyl		163.0	126.7
99	methyl	4-methoxycarbonyl	164.0	152.8
100	ethyl	4-cyano	165.5	171.9
101	cyanomethyl		167.0	186.5
102	methyl	2-hydroxymethyl	167.5	148.3
103	vinyl	4-methyl	169.0	160.2
104	isopropyl	4-methoxy	169.5	135.5
105	methyl	4-methyl	173.0	160.3
106	methoxycarbonylmethyl		174.5	160.6

	Cation		mp(°C)	
No.	N-substituent	Other substituents	exp.	calc.
107	propyl	3-carbamoyl	175.0	161.0
108	ethyl	4-dimethylamino	176.0	144.5
109	prop-2-ynyl	4-methyl	178.0	146.2
110	cyanomethyl	4-methyl	179.0	188.1
111	2-fluoroethyl		180.0	168.3
112	methyl	4-acetyl	183.5	158.9
113	allyl	4-(hydroxyiminomethyl)	185.0	142.6
114	hydrazinocarbonylmethyl		185.5	190.5
115	2-oxopropyl		187.0	172.7
116	ethyl	4-carbamoyl	188.0	195.8
117	(E)-2-carboxy-1-ethenyl		188.5	177.0
118	2-propionamido		189.5	192.9
119	(E)-2-carboxy-1-ethenyl	3-methyl	190.5	167.8
120	allyl[1,2]	2-(hydroxyiminomethyl)	192.5	142.6
121	2-oxopropyl[2]	2-methyl	196.0	162.3
122	2-hydroxyethyl	2-(hydroxyiminomethyl)	198.5	138.8
123	cyanomethyl[2]	2,4-dimethyl	199.0	184.7
124	carboxymethyl		199.0	195.0
125	2-carbamoylethyl		199.0	158.3
126	carbamoylmethyl		200.0	225.9

[1] Outliers according to six-descriptor model.
[2] Outliers according to two-descriptor model.

Supporting Information. Table S2. List of all correlations of melting points of pyridinium bromides by heuristic method.

# P	R^2	R^2_{cv}	F		X + ΔX	t-test	name of the descriptor
1	0.6028	0.5927	186.65	0	$(2.15 \pm 0.08)\cdot 10^2$	27.4158	intercept
				1	$-(4.08 \pm 0.30)\cdot 10$	-13.6620	f-average complementary information content (order 0)
2	0.7125	0.7002	151.16	0	$-(1.91 \pm 0.20)\cdot 10^2$	-9.6301	intercept
				1	$(6.74 \pm 0.45)\cdot 10$	15.0260	total entropy (300K)/# of atoms
				2	$(2.84 \pm 0.42)\cdot 10^3$	6.8270	average nucleophilic reactivity index for a N atom
3	0.7307	0.7147	109.45	0	$-(3.23 \pm 1.06)\cdot 10^3$	-3.0433	intercept
				1	$(6.65 \pm 0.44)\cdot 10$	15.2040	total entropy (300K) /# of atoms
				2	$(2.63 \pm 0.41)\cdot 10^3$	6.3928	average nucleophilic reactivity index for a N atom
				3	$(7.94 \pm 2.77)\cdot 10^2$	2.8630	min valency of a C atom
4	0.7434	0.7210	86.91	0	$(3.22 \pm 0.34)\cdot 10$	9.4023	intercept
				1	-4.36 ± 0.28	-15.7723	f-average complementary information content (order 0)
				2	$(2.29 \pm 0.40)\cdot 10^2$	5.6577	average nucleophilic reactivity index for a N atom
				3	-1.29 ± 0.30	-4.3280	f-number of rings
				4	-2.98 ± 0.81	-3.6709	average information content (order 2)
5	0.7728	0.7503	80.94	0	$(3.97 \pm 0.39)\cdot 10^2$	10.2457	intercept
				1	$-(4.62 \pm 0.29)\cdot 10^1$	-15.8945	f-average complementary information content (order 0)

# P	R^2	R^2_{cv}	F		X + ΔX	t-test	name of the descriptor
				2	$(2.34 \pm 0.38)\cdot 10^{3}$	6.1294	average nucleoph. react. index for a N atom
				3	$-(2.02+0.38)\cdot 10^{2}$	-5.2768	f-relative number of rings
				4	$-(4.11 \pm 0.83)\cdot 10^{1}$	-4.9634	average information content (order 2)
				5	$-(3.66 \pm 0.90)\cdot 10^{-1}$	-4.0782	lowest normal mode vib. frequency
6	0.7883	0.7624	73.24	0	$(8.25 \pm 1.50)\cdot 10^{2}$	5.5036	intercept
				1	-4.79 ± 0.29	-16.6574	f-average complementary information content (order
				2	$(2.21 \pm 0.37)\cdot 10^{2}$	5.9478	average nucleophilic reactivity index for a N atom
				3	-4.48 ± 0.81	-5.5184	average information content (order 2)
				4	$-(3.69 \pm 0.87)\cdot 10^{2}$	-4.2365	lowest normal mode vibrational frequency
				5	$-(1.60 \pm 0.40)\cdot 10^{1}$	-4.0163	f-relative number of rings
				6	$-(1.15 \pm 0.39)\cdot 10^{1}$	-2.9450	min. coulombic interaction for a C-H bond
7	0.8059	0.7757	69.38	0	$(2.42 \pm 0.44)\cdot 10^{3}$	5.4960	intercept
				1	$-(3.42 \pm 0.34)\cdot 10$	-10.1064	f-average complementary information content (order 0)
				2	$(1.78 \pm 0.37)\cdot 10^{3}$	4.7850	average nucleophilic reactivity index for a N atom
				3	$-(1.13 \pm 0.28)\cdot 10$	-4.0119	f-number of rings
				4	$-(2.95 \pm 0.50)\cdot 10$	-5.9580	f-average information content (order 2)
				5	$-(4.31 \pm 0.90)\cdot 10^{-1}$	-4.7877	lowest normal mode vibrational frequency
				6	$-(1.61 \pm 0.39)\cdot 10^{3}$	-4.1742	f-average valency of a H atom

# P	R^2	R^2_{cv}	F		X + ΔX	t-test	name of the descriptor
				7	$-(1.54 \pm 0.39)\cdot10^{2}$	-3.9851	minimum coulombic interaction for a C-H bond
8	0.8284	0.7928	70.02	0	$(2.01 \pm 0.23)\cdot10^{2}$	8.5941	intercept
				1	$-(4.37 \pm 0.27)\cdot10$	-15.9048	f-average complementary information content (order 0)
				2	$(4.11 \pm 5.53)\cdot10^{2}$	7.4394	average nucleophilic reactivity index for a N atom
				3	$(1.06 \pm 0.34)\cdot10^{-2}$	3.1457	f-Kier flexibility index
				4	$-(3.32 \pm 0.61)\cdot10^{-1}$	-5.3990	max. e-n attraction for a N atom
				5	$-(1.70 \pm 0.33)\cdot10^{1}$	-5.0691	min. coulombic interaction for a C-H bond
				6	$-(4.38 \pm 0.76)\cdot10$	-5.7916	average information content (order 2)
				7	$-(3.35 \pm 0.78)\cdot10^{-2}$	-4.3051	lowest normal mode vibrational frequency
				8	$(5.90 \pm 1.46)\cdot10^{-1}$	4.0488	HA dependent HDSA-1
9	0.8433	0.8100	68.75	0	$(1.45 \pm 0.14)\cdot10^{3}$	10.0907	intercept
				1	$-(6.07 \pm 0.60)\cdot10$	-10.0530	average complementary information content (order 0)
				2	$-(5.36 \pm 0.79)\cdot10$	-6.7562	average information content (order 2)
				3	$(1.96 \pm 0.35)\cdot10^{3}$	5.5439	average nucleophilic reactivity index for a N atom
				4	$-(3.80 \pm 0.46)\cdot10^{2}$	-8.3312	FPSA-1 fractional PPSA (PPSA-1/TMSA) [Zefirov
				5	$-(2.06 \pm 0.35)\cdot10^{2}$	-5.8929	min. coulombic interaction for a C-H bond
				6	$(1.29 \pm 0.21)\cdot10$	5.9806	PPSA-3 atomic charge weighted PPSA
				7	$(1.15 \pm 0.29)\cdot10$	3.9518	WNSA-3 weighted PNSA (PNSA3*TMSA/1000)

# P	R^2	R^2_{cv}	F		X + ΔX	t-test	name of the descriptor
				8	$-(2.99 \pm 0.76)\cdot10^{-1}$	-3.9330	lowest normal mode vibrational frequency
				9	$(3.07 \pm 0.80)\cdot10^{3}$	3.8165	min. nucleophilic reactivity index for a N atom
10	0.8491	0.8103	64.17	0	$(3.18 \pm 0.45)\cdot10^{3}$	7.0001	intercept
				1	$-(2.86 \pm 0.33)\cdot10$	-8.5756	f-average complementary information content
				2	$(4.25 \pm 0.55)\cdot10^{3}$	7.6893	average nucleophilic reactivity index for a N atom
				3	$(1.29 \pm 0.32)\cdot10^{-1}$	4.0844	f-Kier flexibility index
				4	$-(3.14 \pm 0.58)\cdot10$	-5.3909	max. e-n attraction for a N atom
				5	$-(1.87 \pm 0.33)\cdot10^{2}$	-5.6233	min. coulombic interaction for a C-H bond
				6	$-(1.45 \pm 0.36)\cdot10^{3}$	-4.0431	f-average valency of a H atom
				7	$-(2.40 \pm 0.45)\cdot10^{1}$	-5.2730	f-average information content (order 2)
				8	$-(4.29 \pm 0.81)\cdot10^{-1}$	-5.2841	lowest normal mode vibrational frequency
				9	$-(1.13 \pm 0.34)\cdot10^{3}$	-3.3220	min. partial charge for a N atom
				10	$(5.26 \pm 1.71)\cdot10$	3.0714	FHBSA fractional HBSA (HBSA/TMSA)
11	0.8505	0.8070	58.42	0	$(4.19 \pm 0.72)\cdot10^{3}$	5.8458	intercept
				1	$-(3.56 \pm 0.43)\cdot10$	-8.2357	f-average complementary information content
				2	$(3.69 \pm 0.57)\cdot10^{3}$	6.5033	average nucleophilic reactivity index for a N atom
				3	$-(1.07 \pm 4.14)\cdot10$	-0.2586	f-relative number of rings
				4	$-(4.65 \pm 0.73)\cdot10$	-6.3818	average information content (order 2)

# P	R^2	R^2_{cv}	F		X + ΔX	t-test	name of the descriptor
				5	$-(3.76 \pm 0.77)\cdot10^{-1}$	-4.8676	lowest normal mode vibrational frequency
				6	$-(1.76 \pm 0.36)\cdot10^{2}$	-4.8874	min. coulombic interaction for a C-H bond
				7	$-(5.15 \pm 1.14)\cdot10^{2}$	-4.4989	f-min. valency of a H atom
				8	-4.22 ± 0.74	-5.7335	max. e-n attraction for a N atom
				9	$-(1.29 \pm 0.30)\cdot10^{3}$	-4.2628	average electrophilic reactivity index for a N atom
				10	$-(1.17 \pm 0.35)\cdot10^{3}$	-3.3083	min. partial charge for a N atom
				11	$-(3.71 \pm 1.49)\cdot10^{2}$	-2.4958	f-average valency of a C atom