Supporting Information for

Prediction of the phase transition temperatures of functional nanostructured liquid crystals: machine learning method based on small data for the design of self-assembled materials

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Table of contents:

1. **Experimental section**----------S4
2. **Training and test dataset**----------S5

Scheme S1 Molecular structures of the cationic moieties of the ionic liquid crystals in the training dataset----------S5

Scheme S2 Molecular structures of the cationic moieties of the ionic liquid crystals in the test dataset----------S6

Scheme S3 Molecular structures of the aliphatic moieties of the ionic liquid crystals in the dataset----------S7

Scheme S4 Molecular structures of the terminal moieties of the ionic liquid crystals in the dataset----------S7

Scheme S5 Molecular structures of the anionic moieties of the ionic liquid crystals in the dataset----------S7

Table S1 Ionic liquid crystals in the training dataset----------S8

Table S2 Ionic liquid crystals in the test dataset----------S10

Table S3 SMILES codes of ionic liquid crystals in the training dataset-------S11

Table S4 SMILES codes of ionic liquid crystals in the test dataset----------S13

3. **Correlation coefficients between explanatory variables**----------S14

Fig. S1 Correlations among the explanatory variables of the ionic liquid crystals in the training dataset----------S14

4. **Five-fold cross validation**----------S15

Table S5 Coefficients of explanatory variables of the five constructed models in the five-fold cross validation----------S15

Table S6 RMSE values for the training and test data in the five-fold cross

validation----------S15

Fig. S2 Relationship between the measured and predicted isotropization temperatures in the five-fold cross validation for the training data and test data----------S16

5. References----------S17

1. Experimental section

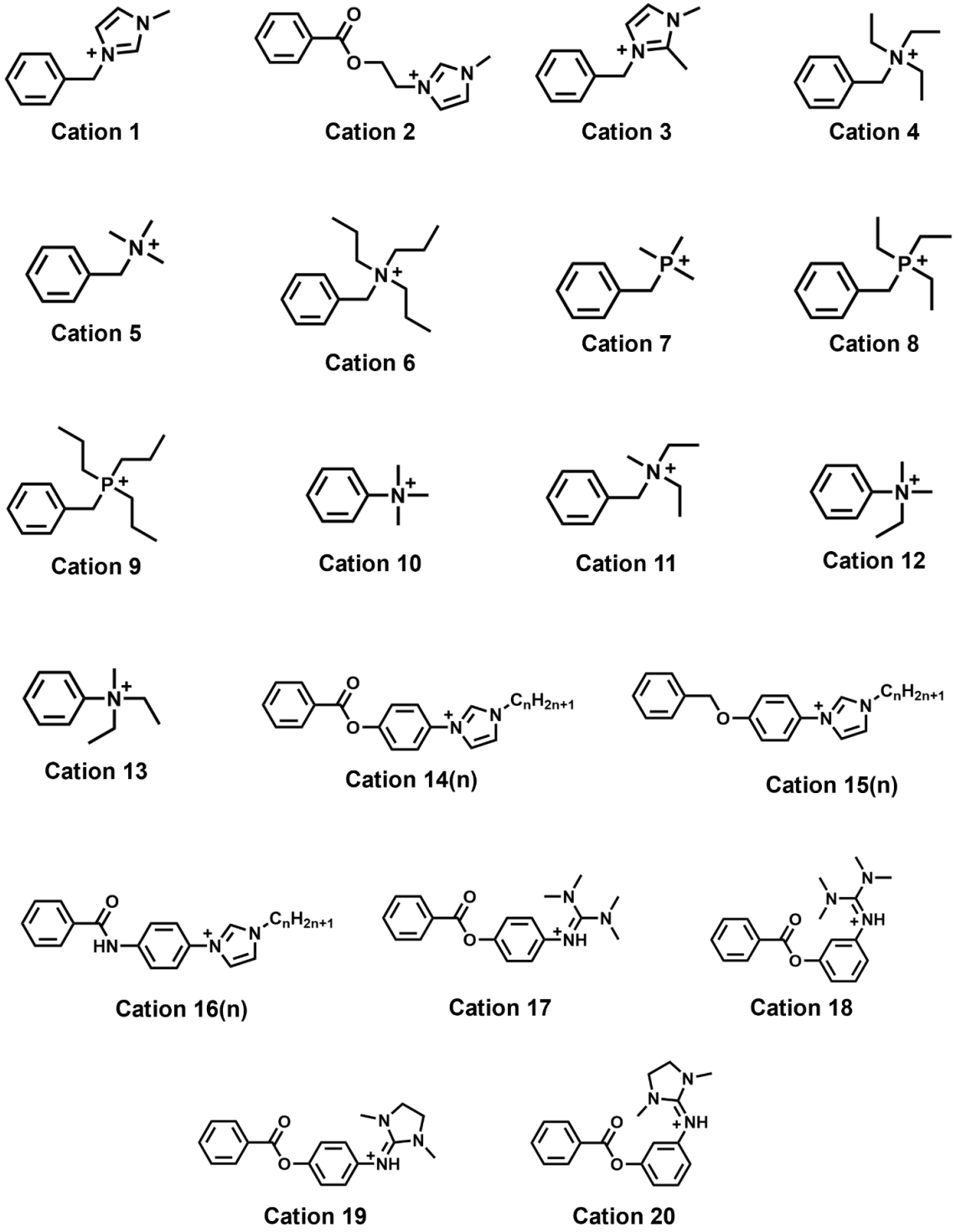
Data preparation

The phase transition temperatures of ILCs were collected from literature.[a-w] The molecular structures of ILCs were manually divided into four parts, namely aliphatic, cationic, terminal, and anionic moieties. The explanatory variables of each moiety were calculated by Spartan' 18. The three-dimensional models of molecules were constructed in Spartan' 18 software and the structures were optimized by the Merck molecular force field (MMFF) and then DFT (B3LYP/6-31G(d,p)). The values of explanatory variables were calculated based on the optimized structures on Spartan' 18.

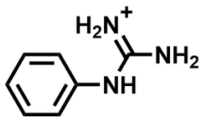
Exhaustive search with linear regression (ES-LiR) analysis

ES-LiR analysis was implemented by Python 3.7.16. The linear regression models were constructed by all combinations of x_n (2^{15}–1). The coefficients of all the constructed models were visualized in the weight diagram with sorting in the ascending order of the CVE value. Each column represents the model constructed. The color of each explanatory variable indicates the magnitude of coefficients in the regression models for all training dataset. The explanatory variables that were not used in the regression are shown in white.

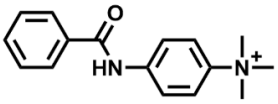
2. Training and test dataset



Scheme S1 Molecular structures of the cationic moieties of the ionic liquid crystals in the training dataset.



Cation 21



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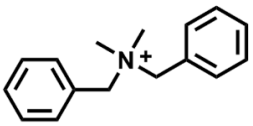

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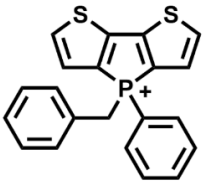

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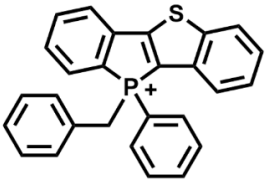

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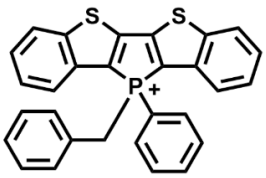

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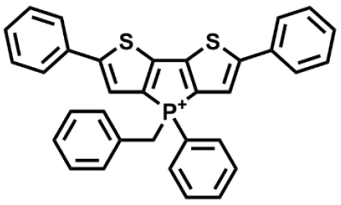

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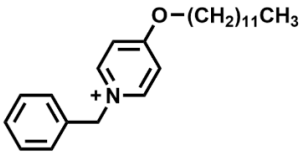

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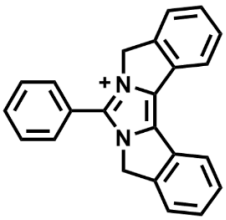

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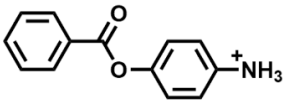

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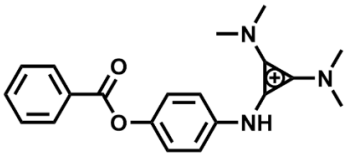

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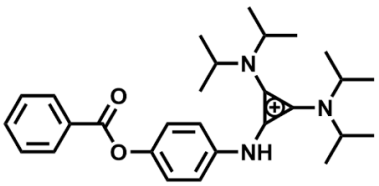

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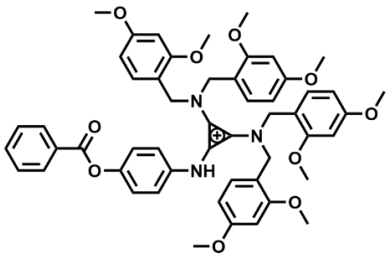
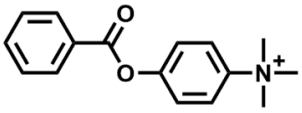


Cation 33



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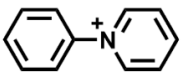
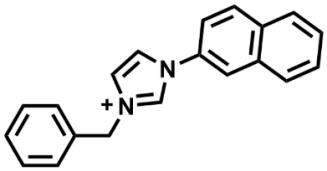
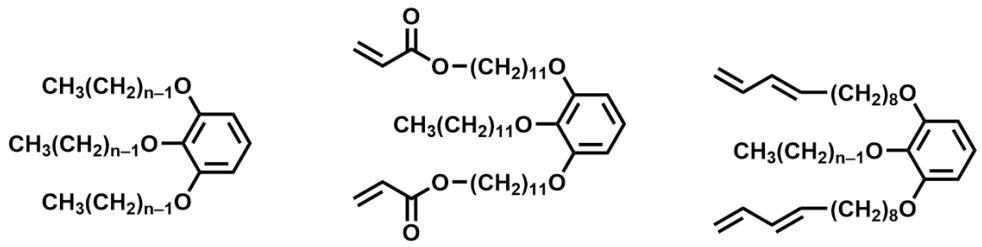


Cation 35

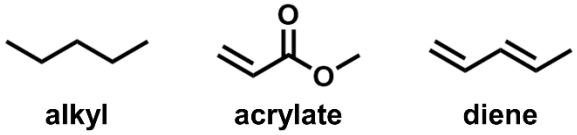


Cation 36

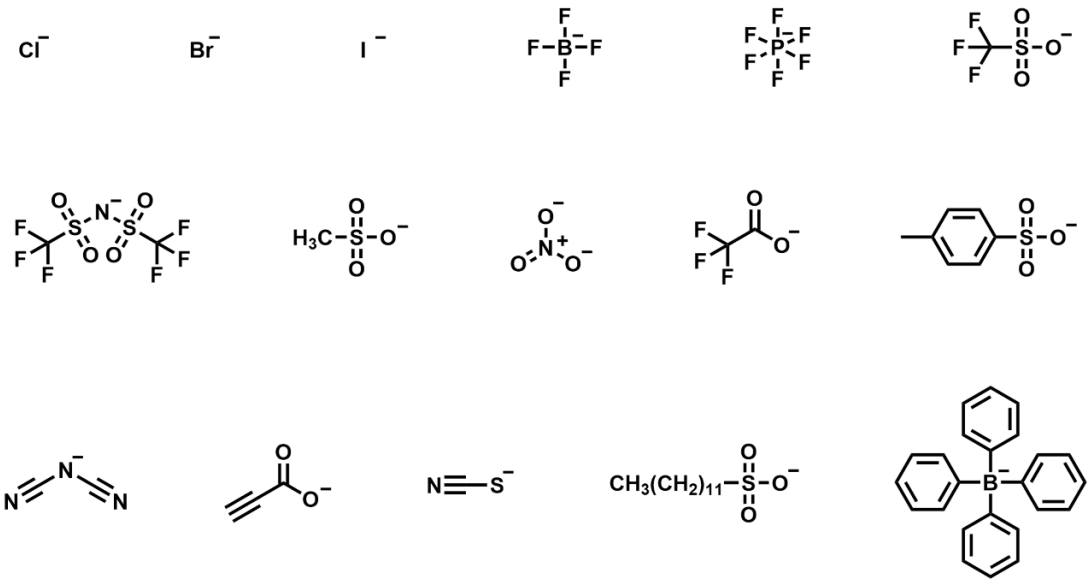
Scheme S2 Molecular structures of the cationic moieties of the ionic liquid crystals in the test dataset.



Scheme S3 Molecular structures of the aliphatic moieties of the ionic liquid crystals in the dataset.



Scheme S4 Molecular structures of the terminal moieties of the ionic liquid crystals in the dataset.



Scheme S5 Molecular structures of the anionic moieties of the ionic liquid crystals in the dataset.

Table S1 Ionic liquid crystals in the training dataset

No.	Aliphatic moiety	Cationic moiety	Anionic moiety	Terminal moiety	T_{iso} (°C)	Type of cationic moiety	Reference
1	Aliphatic **1**(8)	Cation **1**	BF_4^-	Alkyl	133	Imidazolium	a
2	Aliphatic **1**(12)	Cation **1**	BF_4^-	Alkyl	183	Imidazolium	a
3	Aliphtic **2**	Cation **2**	BF_4^-	Acrylate	50	Imidazolium	b
4	Aliphtic **2**	Cation **1**	BF_4^-	Acrylate	5	Imidazolium	b
5	Aliphatic **1**(6)	Cation **1**	BF_4^-	Alkyl	32	Imidazolium	c
6	Aliphatic **1**(10)	Cation **1**	BF_4^-	Alkyl	162	Imidazolium	c
7	Aliphatic **1**(14)	Cation **1**	BF_4^-	Alkyl	185	Imidazolium	c
8	Aliphatic **1**(16)	Cation **1**	BF_4^-	Alkyl	177	Imidazolium	c
9	Aliphatic **1**(18)	Cation **1**	BF_4^-	Alkyl	148	Imidazolium	c
10	Aliphatic **1**(8)	Cation **1**	PF_6^-	Alkyl	78	Imidazolium	d
11	Aliphatic **1**(12)	Cation **1**	PF_6^-	Alkyl	151	Imidazolium	d
12	Aliphatic **1**(16)	Cation **1**	PF_6^-	Alkyl	167	Imidazolium	d
13	Aliphatic **1**(18)	Cation **1**	PF_6^-	Alkyl	161	Imidazolium	d
14	Aliphatic **1**(8)	Cation **1**	OTf^-	Alkyl	1	Imidazolium	d
15	Aliphatic **1**(12)	Cation **1**	OTf^-	Alkyl	63	Imidazolium	d
16	Aliphatic **1**(16)	Cation **1**	OTf^-	Alkyl	117	Imidazolium	d
17	Aliphatic **1**(18)	Cation **1**	OTf^-	Alkyl	119	Imidazolium	d
18	Aliphatic **1**(8)	Cation **1**	$TFSI^-$	Alkyl	2	Imidazolium	d
19	Aliphatic **1**(12)	Cation **1**	$TFSI^-$	Alkyl	37	Imidazolium	d
20	Aliphatic **1**(16)	Cation **1**	$TFSI^-$	Alkyl	60	Imidazolium	d
21	Aliphatic **1**(18)	Cation **1**	$TFSI^-$	Alkyl	77	Imidazolium	d
22	Aliphatic **1**(12)	Cation **3**	BF_4^-	Alkyl	174	Imidazolium	d
23	Aliphatic **1**(12)	Cation **3**	PF_6^-	Alkyl	155	Imidazolium	d
24	Aliphatic **1**(12)	Cation **3**	OTf^-	Alkyl	85	Imidazolium	d
25	Aliphatic **1**(12)	Cation **3**	TFSI	Alkyl	51	Imidazolium	d
26	Aliphatic **1**(10)	Cation **4**	BF_4^-	Alkyl	82	Ammonium	e
27	Aliphatic **1**(12)	Cation **4**	BF_4^-	Alkyl	126	Ammonium	e
28	Aliphatic **1**(14)	Cation **4**	BF_4^-	Alkyl	142	Ammonium	e
29	Aliphatic **3**(12)	Cation **4**	BF_4^-	Diene	19	Ammonium	f
30	Aliphatic **2**	Cation **4**	BF_4^-	Acrylate	2	Ammonium	f
31	Aliphatic **1**(10)	Cation **5**	BF_4^-	Alkyl	194	Ammonium	g
32	Aliphatic **1**(12)	Cation **5**	BF_4^-	Alkyl	206	Ammonium	g
33	Aliphatic **1**(14)	Cation **5**	BF_4^-	Alkyl	202	Ammonium	g
34	Aliphatic **1**(10)	Cation **6**	BF_4^-	Alkyl	82	Ammonium	g
35	Aliphatic **1**(12)	Cation **6**	BF_4^-	Alkyl	80	Ammonium	g
36	Aliphatic **1**(14)	Cation **6**	BF_4^-	Alkyl	91	Ammonium	g
37	Aliphatic **1**(10)	Cation **7**	BF_4^-	Alkyl	164	Phosphonium	g
38	Aliphatic **1**(12)	Cation **7**	BF_4^-	Alkyl	181	Phosphonium	g
39	Aliphatic **1**(14)	Cation **7**	BF_4^-	Alkyl	164	Phosphonium	g
40	Aliphatic **1**(10)	Cation **8**	BF_4^-	Alkyl	48	Phosphonium	g
41	Aliphatic **1**(12)	Cation **8**	BF_4^-	Alkyl	102	Phosphonium	g
42	Aliphatic **1**(14)	Cation **8**	BF_4^-	Alkyl	127	Phosphonium	g
43	Aliphatic **1**(10)	Cation **9**	BF_4^-	Alkyl	66	Phosphonium	g
44	Aliphatic **1**(12)	Cation **9**	BF_4^-	Alkyl	88	Phosphonium	g
45	Aliphatic **1**(14)	Cation **9**	BF_4^-	Alkyl	93	Phosphonium	g
46	Aliphatic **1**(10)	Cation **4**	PF_6^-	Alkyl	58	Ammonium	g
47	Aliphatic **1**(12)	Cation **4**	PF_6^-	Alkyl	76	Ammonium	g
48	Aliphatic **1**(14)	Cation **4**	PF_6^-	Alkyl	114	Ammonium	g
49	Aliphatic **1**(10)	Cation **4**	OTf^-	Alkyl	45	Ammonium	g
50	Aliphatic **1**(12)	Cation **4**	OTf^-	Alkyl	64	Ammonium	g
51	Aliphatic **1**(14)	Cation **4**	OTf^-	Alkyl	65	Ammonium	g
52	Aliphatic **1**(12)	Cation **10**	BF_4^-	Alkyl	196	Ammonium	h
53	Aliphatic **1**(12)	Cation **10**	PF_6^-	Alkyl	168	Ammonium	h
54	Aliphatic **3**(14)	Cation **4**	BF_4^-	Diene	28	Ammonium	i
55	Aliphatic **3**(10)	Cation **11**	BF_4^-	Diene	55	Ammonium	j
56	Aliphatic **3**(12)	Cation **11**	BF_4^-	Diene	62	Ammonium	j
57	Aliphatic **1**(8)	Cation **10**	BF_4^-	Alkyl	161	Ammonium	k
58	Aliphatic **1**(9)	Cation **10**	BF_4^-	Alkyl	173	Ammonium	k

No.	Aliphatic moiety	Cationic moiety	Anionic moiety	Terminal moiety	T_{iso} (°C)	Type of cationic moiety	Reference
59	Aliphatic **1**(10)	Cation **10**	BF_4^-	Alkyl	187	Ammonium	k
60	Aliphatic **1**(11)	Cation **10**	BF_4^-	Alkyl	192	Ammonium	k
61	Aliphatic **1**(13)	Cation **10**	BF_4^-	Alkyl	197	Ammonium	k
62	Aliphatic **1**(14)	Cation **10**	BF_4^-	Alkyl	196	Ammonium	k
63	Aliphatic **1**(12)	Cation **10**	OTf^-	Alkyl	103	Ammonium	k
64	Aliphatic **1**(12)	Cation **12**	BF_4^-	Alkyl	147	Ammonium	k
65	Aliphatic **1**(12)	Cation **12**	PF_6^-	Alkyl	104	Ammonium	k
66	Aliphatic **1**(12)	Cation **12**	OTf	Alkyl	76	Ammonium	k
67	Aliphatic **1**(12)	Cation **13**	BF_4^-	Alkyl	101	Ammonium	k
68	Aliphatic **1**(12)	Cation **13**	PF_6^-	Alkyl	91	Ammonium	k
69	Aliphatic **1**(12)	Cation **13**	OTf^-	Alkyl	83	Ammonium	k
70	Aliphatic **1**(12)	Cation **14**(4)	Br^-	Alkyl	124	Imidazolium	l
71	Aliphatic **1**(12)	Cation **14**(8)	Br^-	Alkyl	76	Imidazolium	l
72	Aliphatic **1**(12)	Cation **14**(14)	Br^-	Alkyl	65	Imidazolium	l
73	Aliphatic **1**(14)	Cation **14**(3)	Br^-	Alkyl	178	Imidazolium	l
74	Aliphatic **1**(14)	Cation **14**(4)	Br^-	Alkyl	120	Imidazolium	l
75	Aliphatic **1**(14)	Cation **14**(14)	Br^-	Alkyl	78	Imidazolium	l
76	Aliphatic **1**(16)	Cation **14**(3)	Br^-	Alkyl	202	Imidazolium	l
77	Aliphatic **1**(16)	Cation **14**(4)	Br^-	Alkyl	171	Imidazolium	l
78	Aliphatic **1**(16)	Cation **14**(5)	Br^-	Alkyl	118	Imidazolium	l
79	Aliphatic **1**(16)	Cation **14**(6)	Br^-	Alkyl	99	Imidazolium	l
80	Aliphatic **1**(16)	Cation **14**(8)	Br^-	Alkyl	96	Imidazolium	l
81	Aliphatic **1**(12)	Cation **15**(4)	Br^-	Alkyl	109	Imidazolium	m
82	Aliphatic **1**(12)	Cation **15**(5)	Br^-	Alkyl	98	Imidazolium	m
83	Aliphatic **1**(14)	Cation **15**(2)	Br^-	Alkyl	177	Imidazolium	m
84	Aliphatic **1**(14)	Cation **15**(3)	Br^-	Alkyl	180	Imidazolium	m
85	Aliphatic **1**(14)	Cation **15**(4)	Br^-	Alkyl	133	Imidazolium	m
86	Aliphatic **1**(14)	Cation **15**(5)	Br^-	Alkyl	98	Imidazolium	m
87	Aliphatic **1**(14)	Cation **15**(6)	Br^-	Alkyl	96	Imidazolium	m
88	Aliphatic **1**(16)	Cation **15**(2)	Br^-	Alkyl	217	Imidazolium	m
89	Aliphatic **1**(16)	Cation **15**(3)	Br^-	Alkyl	184	Imidazolium	m
90	Aliphatic **1**(16)	Cation **15**(4)	Br^-	Alkyl	148	Imidazolium	m
91	Aliphatic **1**(16)	Cation **15**(5)	Br^-	Alkyl	97	Imidazolium	m
92	Aliphatic **1**(18)	Cation **15**(3)	Br^-	Alkyl	189	Imidazolium	m
93	Aliphatic **1**(18)	Cation **15**(5)	Br^-	Alkyl	92	Imidazolium	m
94	Aliphatic **1**(12)	Cation **16**(2)	Br^-	Alkyl	183	Imidazolium	m
95	Aliphatic **1**(12)	Cation **16**(3)	Br^-	Alkyl	122	Imidazolium	m
96	Aliphatic **1**(14)	Cation **16**(2)	Br^-	Alkyl	189	Imidazolium	m
97	Aliphatic **1**(14)	Cation **16**(4)	Br^-	Alkyl	127	Imidazolium	m
98	Aliphatic **1**(10)	Cation **17**	OTf^-	Alkyl	80	Guanidinium	n
99	Aliphatic **1**(12)	Cation **17**	OTf^-	Alkyl	123	Guanidinium	n
100	Aliphatic **1**(14)	Cation **17**	OTf^-	Alkyl	146	Guanidinium	n
101	Aliphatic **1**(16)	Cation **17**	OTf^-	Alkyl	156	Guanidinium	n
102	Aliphatic **1**(10)	Cation **18**	OTf^-	Alkyl	55	Guanidinium	n
103	Aliphatic **1**(12)	Cation **18**	OTf^-	Alkyl	94	Guanidinium	n
104	Aliphatic **1**(14)	Cation **18**	OTf^-	Alkyl	108	Guanidinium	n
105	Aliphatic **1**(16)	Cation **18**	OTf^-	Alkyl	117	Guanidinium	n
106	Aliphatic **1**(6)	Cation **19**	OTf^-	Alkyl	67	Guanidinium	n
107	Aliphatic **1**(8)	Cation **19**	OTf^-	Alkyl	79	Guanidinium	n
108	Aliphatic **1**(10)	Cation **19**	OTf^-	Alkyl	103	Guanidinium	n
109	Aliphatic **1**(12)	Cation **19**	OTf^-	Alkyl	144	Guanidinium	n
110	Aliphatic **1**(14)	Cation **19**	OTf^-	Alkyl	163	Guanidinium	n
111	Aliphatic **1**(16)	Cation **19**	OTf^-	Alkyl	167	Guanidinium	n
112	Aliphatic **1**(8)	Cation **20**	OTf^-	Alkyl	17	Guanidinium	n
113	Aliphatic **1**(10)	Cation **20**	OTf^-	Alkyl	64	Guanidinium	n
114	Aliphatic **1**(12)	Cation **20**	OTf^-	Alkyl	104	Guanidinium	n
115	Aliphatic **1**(14)	Cation **20**	OTf^-	Alkyl	121	Guanidinium	n
116	Aliphatic **1**(16)	Cation **20**	OTf^-	Alkyl	131	Guanidinium	n

Table S2 Ionic liquid crystals in the test dataset

No.	Aliphatic moiety	Cationic moiety	Anionic moiety	Terminal moiety	T_{Iso} (°C)	Type of cationic moiety	Reference
test 1	Aliphatic **1**(10)	Cation **21**	$HCCCO_2^-$	Alkyl	93	Guanidinium	o
test 2	Aliphatic **1**(10)	Cation **21**	BF_4^-	Alkyl	173	Guanidinium	o
test 3	Aliphatic **1**(10)	Cation **21**	NO_3^-	Alkyl	140	Guanidinium	o
test 4	Aliphatic **1**(10)	Cation **21**	Cl^-	Alkyl	165	Guanidinium	o
test 5	Aliphatic **1**(14)	Cation **22**	BF_4^-	Alkyl	172	Ammonium	p
test 6	Aliphatic **1**(12)	Cation **23**	Br^-	Alkyl	137	Ammonium	q
test 7	Aliphatic **1**(12)	Cation **24**	Br^-	Alkyl	205	Phosphole	r
test 8	Aliphatic **1**(12)	Cation **24**	BF_4^-	Alkyl	168	Phosphole	r
test 9	Aliphatic **1**(12)	Cation **24**	BPh_4^-	Alkyl	108	Phosphole	r
test 10	Aliphatic **1**(12)	Cation **24**	OTf^-	Alkyl	98	Phosphole	r
test 11	Aliphatic **1**(12)	Cation **25**	Br^-	Alkyl	173	Phosphole	r
test 12	Aliphatic **1**(12)	Cation **25**	BF_4^-	Alkyl	123	Phosphole	r
test 13	Aliphatic **1**(12)	Cation **26**	Br^-	Alkyl	140	Phosphole	r
test 14	Aliphatic **1**(12)	Cation **26**	BF_4^-	Alkyl	129	Phosphole	r
test 15	Aliphatic **1**(12)	Cation **27**	Br^-	Alkyl	150	Phosphole	r
test 16	Aliphatic **1**(12)	Cation **28**	Br^-	Alkyl	108	Pyridinium with alkyl chain	s
test 17	Aliphatic **1**(12)	Cation **28**	NO_3^-	Alkyl	87	Pyridinium with alkyl chain	s
test 18	Aliphatic **1**(12)	Cation **28**	BF_4^-	Alkyl	59	Pyridinium with alkyl chain	s
test 19	Aliphatic **1**(12)	Cation **28**	PF_6^-	Alkyl	80	Pyridinium with alkyl chain	s
test 20	Aliphatic **1**(12)	Cation **29**	BF_4^-	Alkyl	193	π-conjugated imidazolium	t
test 21	Aliphatic **1**(12)	Cation **29**	OTf^-	Alkyl	95	π-conjugated imidazolium	t
test 22	Aliphatic **1**(12)	Cation **29**	BF_4^-	Alkyl	191	π-conjugated imidazolium	t
test 23	Aliphatic **1**(8)	Cation **29**	BF_4^-	Alkyl	205	π-conjugated imidazolium	t
test 24	Aliphatic **1**(12)	Cation **29**	$TFSI^-$	Alkyl	86	π-conjugated imidazolium	t
test 25	Aliphatic **1**(14)	Cation **30**	TFA^-	Alkyl	63	Ammonium	u
test 26	Aliphatic **1**(14)	Cation **31**	BF_4^-	Alkyl	169	Cyclopropenium	u
test 27	Aliphatic **1**(14)	Cation **32**	BF_4^-	Alkyl	121	Cyclopropenium	u
test 28	Aliphatic **1**(14)	Cation **33**	Cl^-	Alkyl	112	Cyclopropenium	u
test 29	Aliphatic **1**(12)	Cation **34**	I^-	Alkyl	139	Ammonium	u
test 30	Aliphatic **1**(12)	Cation **35**	BF_4^-	Alkyl	180	Pyridinium	v
test 31	Aliphatic **1**(10)	Cation **35**	PF_6^-	Alkyl	153	Pyridinium	v
test 32	Aliphatic **1**(12)	Cation **35**	PF_6^-	Alkyl	170	Pyridinium	v
test 33	Aliphatic **1**(14)	Cation **35**	PF_6^-	Alkyl	174	Pyridinium	v
test 34	Aliphatic **1**(12)	Cation **35**	SCN^-	Alkyl	166	Pyridinium	v
test 35	Aliphatic **1**(12)	Cation **35**	$C_{12}H_{25}SO_3^-$	Alkyl	118	Pyridinium	v
test 36	Aliphatic **1**(12)	Cation **35**	OTf^-	Alkyl	105	Pyridinium	v
test 37	Aliphatic **1**(10)	Cation **35**	$TFSI^-$	Alkyl	47	Pyridinium	v
test 38	Aliphatic **1**(12)	Cation **35**	$TFSI^-$	Alkyl	64	Pyridinium	v
test 39	Aliphatic **1**(14)	Cation **35**	$TFSI^-$	Alkyl	69	Pyridinium	v
test 40	Aliphatic **1**(12)	Cation **36**	Cl^-	Alkyl	128	Imidazolium with naphthalene	w
test 41	Aliphatic **1**(12)	Cation **36**	Br^-	Alkyl	120	Imidazolium with naphthalene	w
test 42	Aliphatic **1**(12)	Cation **36**	I^-	Alkyl	103	Imidazolium with naphthalene	w
test 43	Aliphatic **1**(12)	Cation **36**	BF_4^-	Alkyl	100	Imidazolium with naphthalene	w
test 44	Aliphatic **1**(12)	Cation **36**	PF_6^-	Alkyl	80	Imidazolium with naphthalene	w
test 45	Aliphatic **1**(12)	Cation **36**	$TFSI^-$	Alkyl	52	Imidazolium with naphthalene	w

Table S3 SMILES codes of ionic liquid crystals in the training dataset

No.	SMILES code of molecule	SMILES code of anion
1	CCCCCCCCOC1=C(OCCCCCCCCC)C(OCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[B-](F)(F)F
2	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[B-](F)(F)F
3	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCOC(C=C)=O)C=C(C(OCC[N+]2=CN(C)C=C2)=O)C=C1OCCCCCCCCCCCCOC(C=C)=O	F[B-](F)(F)F
4	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCOC(C=C)=O)C=C(C[N+]2=CN(C)C=C2)C=C1OCCCCCCCCCCCCOC(C=C)=O	F[B-](F)(F)F
5	CCCCCCOC1=C(C(OCCCCCC)=CC(C[N+]2=C(N(C=C2)C))=C1)OCCCCCC	F[B-](F)(F)F
6	CCCCCCCCCCOC1=CC(C[N+]2=C(N(C=C2)C))=CC(OCCCCCCCCCC)=C1OCCCCCCCCCC	F[B-](F)(F)F
7	CCCCCCCCCCCCCCOC1=C(C(OCCCCCCCCCCCCCC)=CC(C[N+]2=C(N(C=C2)C))=C1)OCCCCCCCCCCCCCC	F[B-](F)(F)F
8	CCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[B-](F)(F)F
9	CCCCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[B-](F)(F)F
10	CCCCCCCCOC1=C(OCCCCCCCCC)C(OCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[P-](F)(F)(F)(F)F
11	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[P-](F)(F)(F)(F)F
12	CCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[P-](F)(F)(F)(F)F
13	CCCCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	F[P-](F)(F)(F)(F)F
14	CCCCCCCCOC1=C(OCCCCCCCCC)C(OCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([O-])(C(F)(F)F)=O
15	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([O-])(C(F)(F)F)=O
16	CCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([O-])(C(F)(F)F)=O
17	CCCCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([O-])(C(F)(F)F)=O
18	CCCCCCCCOC1=C(OCCCCCCCCC)C(OCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
19	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
20	CCCCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
21	CCCCCCCCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCCCCCC)=CC(C[N+]2=CN(C)C=C2)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
22	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=C(C)N(C)C=C2)=C1	F[B-](F)(F)F
23	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=C(C)N(C)C=C2)=C1	F[P-](F)(F)(F)(F)F
24	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=C(C)N(C)C=C2)=C1	O=S([O-])(C(F)(F)F)=O
25	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+]2=C(C)N(C)C=C2)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
26	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[B-](F)(F)F
27	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[B-](F)(F)F
28	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[B-](F)(F)F
29	CCCCCCCCCCCCOC1=C(OCCCCCCCC/C=C/C=C)C=C(C[N+](CC)(CC)CC)C=C1OCCCCCCCC/C=C/C=C	F[B-](F)(F)F
30	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCOC(C=C)=O)C=C(C[N+](CC)(CC)CC)C=C1OCCCCCCCCCCCCOC(C=C)=O	F[B-](F)(F)F
31	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[N+](C)(C)C)=C1	F[B-](F)(F)F
32	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+](C)(C)C)=C1	F[B-](F)(F)F
33	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[N+](C)(C)C)=C1	F[B-](F)(F)F
34	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[N+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
35	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
36	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[N+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
37	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[P+](C)(C)C)=C1	F[B-](F)(F)F
38	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+](C)(C)C)=C1	F[B-](F)(F)F
39	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[P+](C)(C)C)=C1	F[B-](F)(F)F
40	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[P+](CC)(CC)CC)=C1	F[B-](F)(F)F
41	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+](CC)(CC)CC)=C1	F[B-](F)(F)F
42	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[P+](CC)(CC)CC)=C1	F[B-](F)(F)F
43	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[P+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
44	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
45	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[P+](CCC)(CCC)CCC)=C1	F[B-](F)(F)F
46	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[P-](F)(F)(F)(F)F
47	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[P-](F)(F)(F)(F)F
48	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	F[P-](F)(F)(F)(F)F
49	CCCCCCCCCCOC1=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	O=S([O-])(C(F)(F)F)=O
50	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	O=S([O-])(C(F)(F)F)=O
51	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=CC(C[N+](CC)(CC)CC)=C1	O=S([O-])(C(F)(F)F)=O
52	C[N+](C)(C)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[B-](F)(F)F
53	C[N+](C)(C)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[P-](F)(F)(F)(F)F
54	CCCCCCCCCCCCCCOC1=C(OCCCCCCCCC/C=C/C=C)C=C(C[N+](CC)(CC)CC)C=C1OCCCCCCCC/C=C/C=C	F[B-](F)(F)F
55	C[N+](CC)(CC)CC1=CC(OCCCCCCCC/C=C/C=C)=C(OCCCCCCCCCC)C(OCCCCCCCC/C=C/C=C)=C1	F[B-](F)(F)F
56	C[N+](CC)(CC)CC1=CC(OCCCCCCCC/C=C/C=C)=C(OCCCCCCCCCCCC)C(OCCCCCCCC/C=C/C=C)=C1	F[B-](F)(F)F
57	C[N+](C)(C)C1=CC(OCCCCCCCC)=C(OCCCCCCCC)C(OCCCCCCCC)=C1	F[B-](F)(F)F
58	C[N+](C)(C)C1=CC(OCCCCCCCCC)=C(OCCCCCCCCC)C(OCCCCCCCCC)=C1	F[B-](F)(F)F
59	C[N+](C)(C)C1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1	F[B-](F)(F)F

No.	SMILES code of molecule	SMILES code of anion
60	C[N+](C)(C)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[B-](F)(F)F
61	C[N+](C)(C)C1=CC(OCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=C1	F[B-](F)(F)F
62	C[N+](C)(C)C1=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C1	F[B-](F)(F)F
63	C[N+](C)(C)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	O=S([O-])(C(F)(F)F)=O
64	C[N+](C)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[B-](F)(F)F
65	C[N+](C)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[P-](F)(F)(F)(F)F
66	C[N+](C)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	O=S([O-])(C(F)(F)F)=O
67	C[N+](CC)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[B-](F)(F)F
68	C[N+](CC)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	F[P-](F)(F)(F)(F)F
69	C[N+](CC)(CC)C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1	O=S([O-])(C(F)(F)F)=O
70	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(C(OC2=CC=C([N+]3=CN(CCCC)C=C3)C=C2)=O)C=C1OCCCCCCCCCCCC	[Br-]
71	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(C(OC2=CC=C([N+]3=CN(CCCCCCCC)C=C3)C=C2)=O)C=C1OCCCCCCCCCCCC	[Br-]
72	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(C(OC2=CC=C([N+]3=CN(CCCCCCCCCCCCCC)C=C3)C=C2)=O)C=C1OCCCCCCCCCCC	[Br-]
73	O=C(OC1=CC=C([N+]2=CN(CCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C3	[Br-]
74	O=C(OC1=CC=C([N+]2=CN(CCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C3	[Br-]
75	O=C(OC1=CC=C([N+]2=CN(CCCCCCCCCCCCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C3	[Br-]
76	O=C(OC1=CC=C([N+]2=CN(CCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
77	O=C(OC1=CC=C([N+]2=CN(CCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
78	O=C(OC1=CC=C([N+]2=CN(CCCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
79	O=C(OC1=CC=C([N+]2=CN(CCCCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
80	O=C(OC1=CC=C([N+]2=CN(CCCCCCCC)C=C2)C=C1)C3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
81	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(COC2=CC=C([N+]3=CN(CCCC)C=C3)C=C2)C=C1OCCCCCCCCCCCC	[Br-]
82	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(COC2=CC=C([N+]3=CN(CCCCC)C=C3)C=C2)C=C1OCCCCCCCCCCCC	[Br-]
83	CCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C3	[Br-]
84	CCCCCCCCCCCCCCOC1=CC(COC2=CC=C([N+]3=CN(CCC)C=C3)C=C2)=CC(OCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
85	CCCCCCCCCCCCCCOC1=CC(COC2=CC=C([N+]3=CN(CCCC)C=C3)C=C2)=CC(OCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
86	CCCCCCCCCCCCCCOC1=CC(COC2=CC=C([N+]3=CN(CCCCC)C=C3)C=C2)=CC(OCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
87	CCCCCCCCCCCCCCOC1=CC(COC2=CC=C([N+]3=CN(CCCCC)C=C3)C=C2)=CC(OCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
88	CCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
89	CCCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
90	CCCCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3	[Br-]
91	CCCCCCCCCCCCCCCCCOC1=CC(COC2=CC=C([N+]3=CN(CCCCC)C=C3)C=C2)=CC(OCCCCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
92	CCCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCC)=C3	[Br-]
93	CCCCCN(C=C1)C=[N+]1C2=CC=C(C=C2)OCC3=CC(OCCCCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCC)=C3	[Br-]
94	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(C(NC2=CC=C([N+]3=CN(CC)C=C3)C=C2)=O)C=C1OCCCCCCCCCCCC	[Br-]
95	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C=C(C(NC2=CC=C([N+]3=CN(CCC)C=C3)C=C2)=O)C=C1OCCCCCCCCCCCC	[Br-]
96	CCN(C=C1)C=[N+]1C2=CC=C(C=C2)NC(C3=CC(OCCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C3)=O	[Br-]
97	CCCCCCCCCCCCCCCCCCOC1=CC(C(NC2=CC=C([N+]3=CN(CCCC)C=C3)C=C2)=O)=CC(OCCCCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	[Br-]
98	O=C(C1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C(N(C)C)/N(C)C	FC(F)(F)S(=O)([O-])=O
99	O=C(C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCC)C(OCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C(N(C)C)/N(C)C	FC(F)(F)S(=O)([O-])=O
100	O=C(C1=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C(N(C)C)/N(C)C	FC(F)(F)S(=O)([O-])=O
101	O=C(C1=CC(OCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C(N(C)C)/N(C)C	FC(F)(F)S(=O)([O-])=O
102	O=C(C1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C(N(C)C)/N(C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
103	O=C(C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCC)C(OCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C(N(C)C)/N(C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
104	O=C(C1=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C(N(C)C)/N(C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
105	O=C(C1=CC(OCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C(N(C)C)/N(C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
106	O=C(C1=CC(OCCCCCC)=C(OCCCCCC)C(OCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
107	O=C(C1=CC(OCCCCCCCCC)=C(OCCCCCCCCC)C(OCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
108	O=C(C1=CC(OCCCCCCCCCCC)=C(OCCCCCCCCCCC)C(OCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
109	O=C(C1=CC(OCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
110	O=C(C1=CC(OCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
111	O=C(C1=CC(OCCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+]([H])=C3N(CCN/3C)C	FC(F)(F)S(=O)([O-])=O
112	O=C(C1=CC(OCCCCCCCCC)=C(OCCCCCCCCC)C(OCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C3N(CCN/3C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
113	O=C(C1=CC(OCCCCCCCCCCC)=C(OCCCCCCCCCCC)C(OCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C3N(CCN/3C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
114	O=C(C1=CC(OCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C3N(CCN/3C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
115	O=C(C1=CC(OCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C3N(CCN/3C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O
116	O=C(C1=CC(OCCCCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCCCC)=C1)OC2=CC(/[N+]([H])=C3N(CCN/3C)C)=CC=C2	FC(F)(F)S(=O)([O-])=O

Table S4 SMILES codes of ionic liquid crystals in the test dataset

No.	SMILES code of molecule	SMILES code of anion
test 1	[NH2+]=C(N)NC1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1	[O-]C(C#C)=O
test 2	[NH2+]=C(N)NC1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1	F[B-](F)(F)F
test 3	[NH2+]=C(N)NC1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1	O=N([O-])=O
test 4	[NH2+]=C(N)NC1=CC(OCCCCCCCCCC)=C(OCCCCCCCCCC)C(OCCCCCCCCCC)=C1	[Cl-]
test 5	CCCCCCCCCCCCCCOC(C=C1C(N([H])C2=CC=C([N+](C)(C)C)C=C2)=O)=C(C(OCCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	F[B-](F)(F)F
test 6	CCCCCCCCCCCCOC1=C(C(OCCCCCCCCCCCC)=CC(C[N+](C)(C)CC2=CC=CC=C2)=C1)OCCCCCCCCCCCC	[Br-]
test 7	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C=CS4)=C4C5=C2C=CS5)=C1	[Br-]
test 8	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C=CS4)=C4C5=C2C=CS5)=C1	F[B-](F)(F)F
test 9	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C=CS4)=C4C5=C2C=CS5)=C1	C1([B-](C2=CC=CC=C2)(C3=CC=CC=C3)C4=CC=CC=C4)=CC=CC=C1
test 10	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C=CS4)=C4C5=C2C=CS5)=C1	O=S([O-])(C(F)(F)F)=O
test 11	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C(C=CC=C4)=C4S5)=C5C6=C2C=CC=C6)=C1	[Br-]
test 12	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C(C=CC=C4)=C4S5)=C5C6=C2C=CC=C6)=C1	F[B-](F)(F)F
test 13	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C(C=CC=C4)=C4S5)=C5C6=C2C7=C(C=CC=C7)S6)=C1	[Br-]
test 14	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C(C=CC=C4)=C4S5)=C5C6=C2C7=C(C=CC=C7)S6)=C1	F[B-](F)(F)F
test 15	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C[P+]2(C3=CC=CC=C3)C(C=C(C4=CC=CC=C4)S5)=C5C6=C2C=C(C7=CC=CC=C7)S6)=C1	[Br-]
test 16	CCCCCCCCCCCCOC1=CC=[N+](C=C1)CC2=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C2	[Br-]
test 17	CCCCCCCCCCCCOC1=CC=[N+](C=C1)CC2=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C2	O=N([O-])=O
test 18	CCCCCCCCCCCCOC1=CC=[N+](C=C1)CC2=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C2	F[B-](F)(F)F
test 19	CCCCCCCCCCCCOC1=CC=[N+](C=C1)CC2=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C2	F[P-](F)(F)(F)(F)F
test 20	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C2=[N+]3C(C4=C(C3)C=CC=C4)=C5N2CC6=C5C=CC=C6)=C1	F[B-](F)(F)F
test 21	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C2=[N+]3C(C4=C(C3)C=CC=C4)=C5N2CC6=C5C=CC=C6)=C1	O=S([O-])(C(F)(F)F)=O
test 22	CCCCCCCCCCCCCCCCCOC1=CC(C2=[N+]3C(C4=C(C3)C=CC=C4)=C5N2CC6=C5C=CC=C6)=CC(OCCCCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCCC	F[B-](F)(F)F
test 23	CCCCCCCCOC1=C(OCCCCCCCC)C(OCCCCCCCC)=CC(C2=[N+]3C(C4=C(C3)C=CC=C4)=C5N2CC6=C5C=CC=C6)=C1	F[B-](F)(F)F
test 24	CCCCCCCCCCCCOC1=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=CC(C2=[N+]3C(C4=C(C3)C=CC=C4)=C5N2CC6=C5C=CC=C6)=C1	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
test 25	O=C(OC1=CC=C([NH3+])C=C1)C2=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C2	O=C([O-])C(F)(F)F
test 26	O=C(OC1=CC=C(/[N+](H)=C2C(N(C)C)=C/2N(C)C)C=C1)C3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCC)=C3	F[B-](F)(F)F
test 27	O=C(OC1=CC=C(/[N+](H)=C2C(N(C(C)C)C(C)C)=C/2N(C(C)C)C(C)C)C=C1)C3=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C3	F[B-](F)(F)F
test 28	O=C(C1=CC(OCCCCCCCCCCCCCC)=C(OCCCCCCCCCCCCCC)C(OCCCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)/[N+](H)=C3C(N(CC4=C(OC)C=C(OC)C=C4)CC5=C(OC)C=C(OC)C=C5)=C/3N(CC6=C(OC)C=C(OC)C=C6)CC7=C(OC)C=C(OC)C=C7	[Cl-]
test 29	O=C(C1=CC(OCCCCCCCCCCCC)=C(OCCCCCCCCCCCC)C(OCCCCCCCCCCCC)=C1)OC2=CC=C(C=C2)[N+](C)(C)C	[I-]
test 30	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	F[B-](F)(F)F
test 31	CCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCC)=C1OCCCCCCCCCC	F[P-](F)(F)(F)(F)F
test 32	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	F[P-](F)(F)(F)(F)F
test 33	CCCCCCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCCC	F[P-](F)(F)(F)(F)F
test 34	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	[S-]C#N
test 35	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	CCCCCCCCCCCCS(=O)([O-])=O
test 36	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	O=S([O-])(C(F)(F)F)=O
test 37	CCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCC)=C1OCCCCCCCCCC	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
test 38	CCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCC)=C1OCCCCCCCCCCCC	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
test 39	CCCCCCCCCCCCCCCCOC1=CC([N+]2=CC=CC=C2)=CC(OCCCCCCCCCCCCCC)=C1OCCCCCCCCCCCCCC	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O
test 40	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	[Cl-]
test 41	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	[Br-]
test 42	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	[I-]
test 43	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	F[B-](F)(F)F
test 44	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	F[P-](F)(F)(F)(F)F
test 45	CCCCCCCCCCCCCOC(C=C1C[N+]2=CN(C3=CC(C=CC=C4)=C4C=C3)C=C2)=C(C(OCCCCCCCCCCCCC)=C1)OCCCCCCCCCCCCC	O=S([N-]S(=O)(C(F)(F)F)=O)(C(F)(F)F)=O

3. Correlation coefficients between explanatory variables

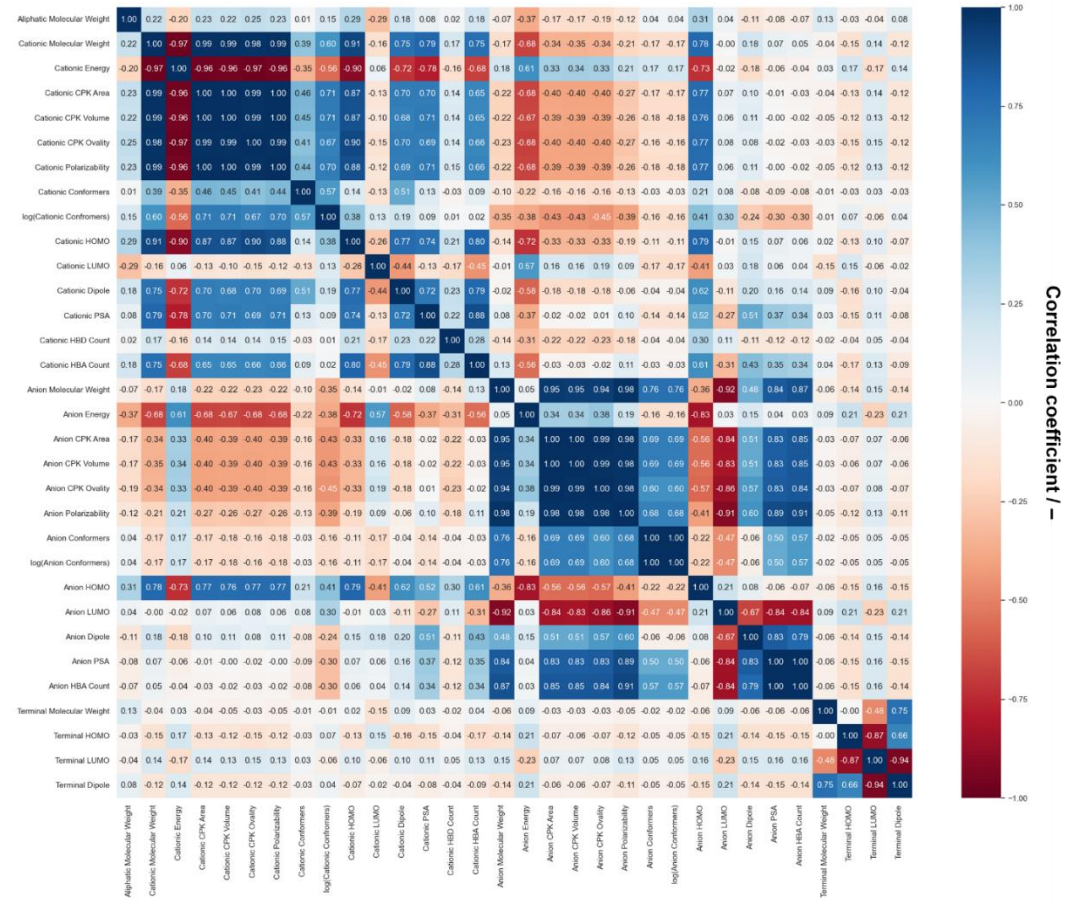


Fig. S1 Correlations among the explanatory variables of the ionic liquid crystals in the training dataset.

4. Five-fold cross validation

In five-fold cross validation, the dataset was randomly divided into five groups. Five models were constructed using four groups as training data. The prediction accuracy of the five models was evaluated by remaining one group as test data. The average of the RMSE values for test data was regarded as cross-validation error. Table S3, S4, and Figure S2 shows the results of the five-fold cross validation when using the selected seven descriptors as follow, aliphatic molecular weight (x_1), cationic molecular weight (x_2), log(cationic conformers) (x_9), cationic dipole (x_{12}), anion molecular weight (x_{16}), anion dipole (x_{26}), and terminal dipole (x_{33}).

Table S5 Coefficients of explanatory variables of the five constructed models in the five-fold cross validation

Explanatory variables	No.1	No.2	No.3	No.4	No.5
Aliphatic MolecularWeight	22.7	20.7	17.0	20.2	18.6
Cationic Molecular Weight	–9.0	–9.0	–14.2	–13.6	–12.9
log(Cationic Conformers)	–28.8	–32.6	–28.7	–26.4	–27.7
Cationic Dipole	16.2	18.1	21.1	19.7	19.1
Anion Molecular Weight	–30.9	–29.2	–29.8	–27.5	–28.6
Anion Dipole	–6.2	–10.0	–9.1	–10.7	–9.1
Terminal Dipole	–28.6	–23.9	–25.4	–28.5	–26.4

Table S6 RMSE values for the training and test data in the five-fold cross validation

	No.1	No.2	No.3	No.4	No.5	average
RMSE for training data / °C	21.4	24.0	22.8	24.0	24.8	23.4
RMSE for test data / °C	32.9	24.0	28.1	23.6	18.7	25.5

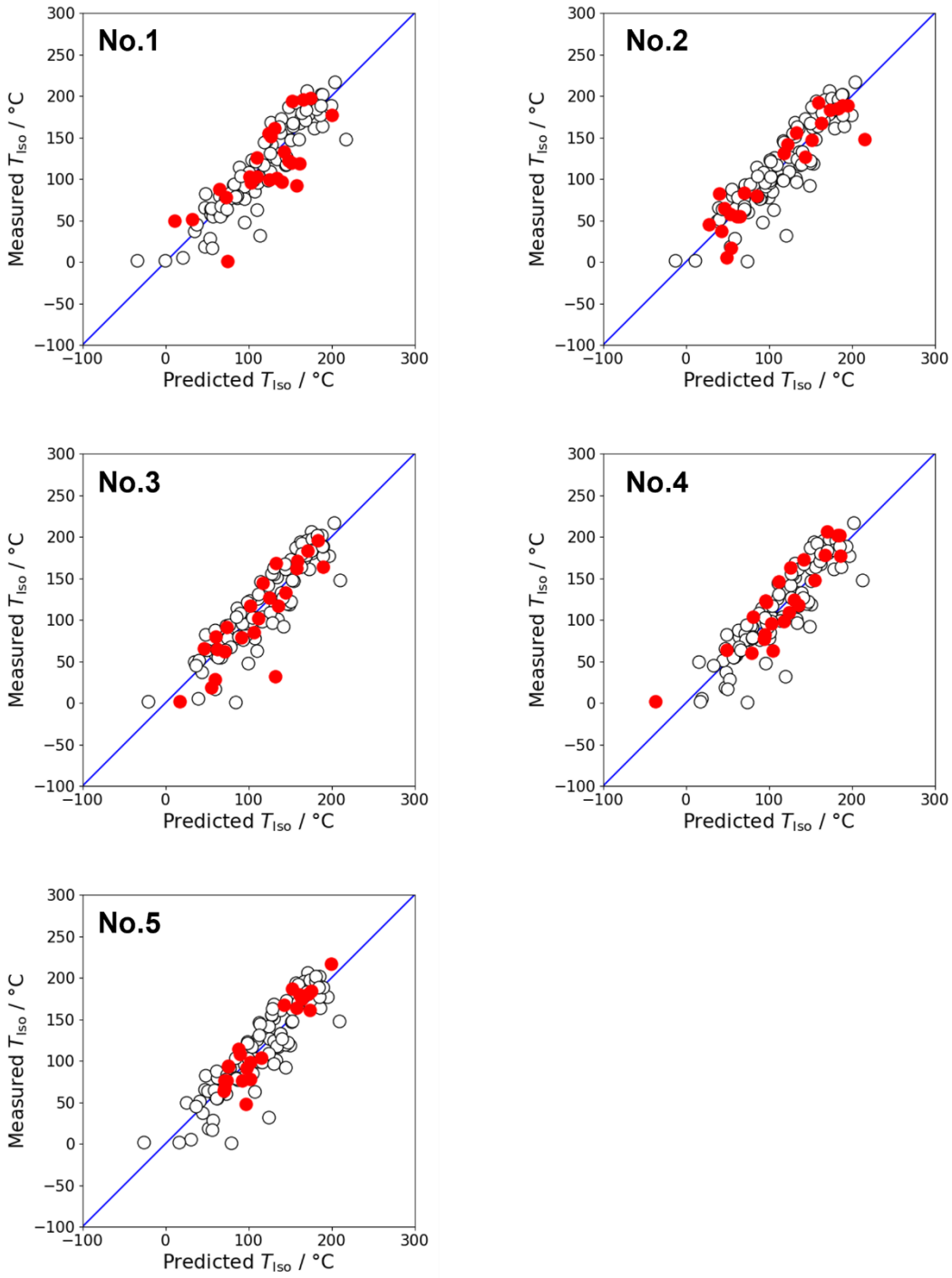


Fig. S2 Relationship between the measured and predicted isotropization temperatures (T_{Iso}s) in the five-fold cross validation for the training data (white circle) and test data (red circle).

5. References

a. M. Yoshio, T. Mukai, H. Ohno and T. Kato, *J. Am. Chem. Soc.*, 2004, **126**, 994–995.

b. M. Yoshio, T. Kagata, K. Hoshino, T. Mukai, H. Ohno and T. Kato, *J. Am. Chem. Soc.*, 2006, **128**, 5570–5577.

c. M. Yoshio, T. Mukai, H. Ohno and T. Kato, in *ACS Symposium Series*, ed. J. F. Brennecke, R. D. Rogers and K. R. Seddon, American Chemical Society, WA, 2007, vol. 975, ch. 11, pp. 161–171.

d. M. Yoshio, T. Ichikawa, H. Shimura, T. Kagata, A. Hamasaki, T. Mukai, H. Ohno and T. Kato, *Bull. Chem. Soc. Jpn.*, 2007, **80**, 1836–1841.

e. T. Ichikawa, M. Yoshio, A. Hamasaki, T. Mukai, H. Ohno and T. Kato, *J. Am. Chem. Soc.*, 2007, **129**, 10662–10663.

f. T. Ichikawa, M. Yoshio, A. Hamasaki, J. Kagimoto, H. Ohno and T. Kato, *J. Am. Chem. Soc.*, 2011, **133**, 2163–2169.

g. T. Ichikawa, M. Yoshio, A. Hamasaki, S. Taguchi, F. Liu, X.-B. Zeng, G. Ungar, H. Ohno and T. Kato, *J. Am. Chem. Soc.*, 2012, **134**, 2634–2643.

h. B. Soberats, M. Yoshio, T. Ichikawa, X. Zeng, H. Ohno, G. Ungar and T. Kato, *J. Am. Chem. Soc.*, 2015, **137**, 13212–13215.

i. N. Marets, D. Kuo, J. R. Torrey, T. Sakamoto, M. Henmi, H. Katayama and T. Kato, *Adv. Healthcare Mater.*, 2017, **6**, 1700252.

j. T. Sakamoto, T. Ogawa, H. Nada, K. Nakatsuji, M. Mitani, B. Soberats, K. Kawata, M. Yoshio, H. Tomioka, T. Sasaki, M. Kimura, M. Henmi and T. Kato, *Adv. Sci.*, 2017, **5**, 1700405.

k. D. Kuo, B. Soberats, K. R. S. Kumar, M. Yoshio, T. Ichikawa, H. Ohno, X. Zeng, G. Ungar and T. Kato, *Mol. Syst. Des. Eng.*, 2019, **4**, 342–347.

l. X. Cheng, X. Bai, S. Jing, H. Ebert, M. Prehm and C. Tschierske, *Chem. Eur. J.*, 2010, **16**, 4588–4601.

m. X. Cheng, F. Su, R. Huang, H. Gao, M. Prehm and C. Tschierske, *Soft Matter*, 2012, **8**, 2274–2285.

n. M. Butschies, J. C. Haenle, S. Tussetschläger and S. Laschat, *Liq. Cryst.*, 2013, **40**, 52–71.

o. D. Kim, S. Jon, H.-K. Lee, K. Baek, N.-K. Oh, W.-C. Zin and K. Kim, *Chem. Commun.*, 2005, 5509–5511.

p. F. Camerel, G. Ulrich, J. Barberá and R. Ziessel, *Chem. Eur. J.*, 2007, **13**, 2189–2200.

q. R. van de Coevering, P. C. A. Bruijnincx, C. A. van Walree, R. J. M. K. Gebbink and G. van

Koten, *Eur. J. Org. Chem.*, 2007, **2007**, 2931–2939.

r. Y. Ren, W. H. Kan, M. A. Henderson, P. G. Bomben, C. P. Berlinguette, V. Thangadurai and T. Baumgartner, *J. Am. Chem. Soc.*, 2011, **133**, 17014–17026.

s. A. Pană, F. L. Badea, M. Ilis, T. Staicu, M. Micutz, I. Pasuk and V. Cîrcu, *J. Mol. Struct.*, 2015, **1083**, 245–251.

t. K. Takagi, K. Yamauchi, S. Kubota, S. Nagano, M. Hara, T. Seki, K. Murakami, Y. Ooyama, J. Ohshita, M. Kondo and H. Masu, *RSC Adv.*, 2016, **6**, 9152–9159.

u. J. Litterscheidt, J. S. Bandar, M. Ebert, R. Forschner, K. Bader, T. H. Lambert, W. Frey, A. Bühlmeyer, M. Brändle, F. Schulz and S. Laschat, *Angew. Chem. Int. Ed.*, 2020, **59**, 10557–10565.

v. R.-T. Wang, S.-J. J. Tsai, G.-H. Lee and C. K. Lai, *Dyes Pigments*, 2020, **173**, 107913.

w. N. del Giudice, M. L'Her, E. Scrafton, Y. Atoini, G. Gentile, B. Heinrich, R. Berthiot, A. Aliprandi and L. Douce, *Eur. J. Org. Chem.*, 2021, **2021**, 2091–2098.