

Supporting Information

Table S1. The performance metrics of DL-model that applied to different testing sets which based on 137 molecular features/descriptors. N is the sample size of the dataset. For RMSE, the unit is in Kelvin (K).

System	Test		
	N	RMSE	R ²
Cluster 1	605	30.99	0.94
Cluster 2	134	34.18	0.64
Cluster 3	186	32.57	0.62
Cluster 4	31	29.32	0.63
Cluster 5	297	35.88	0.56
Entire Dataset	1253	32.88	0.90

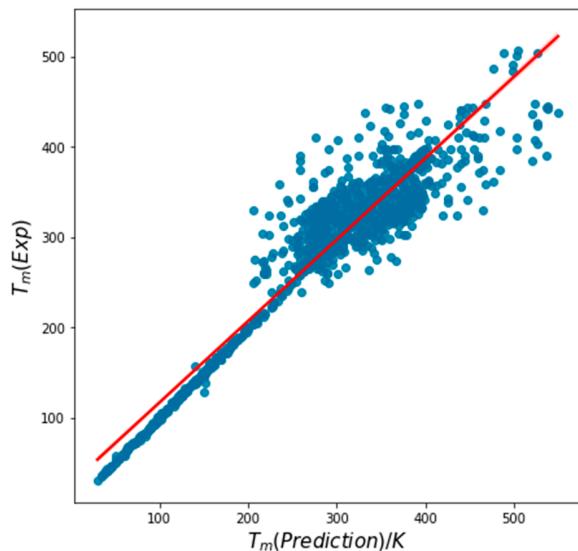


Figure S1. DL model predicted melting point (i.e. T_m (Prediction)/K) values (in blue color) of the entire ILs dataset versus the experimental measured melting point (i.e. T_m (Exp)/K) (in red color) obtained from the literatures (i.e. ILThermo database).

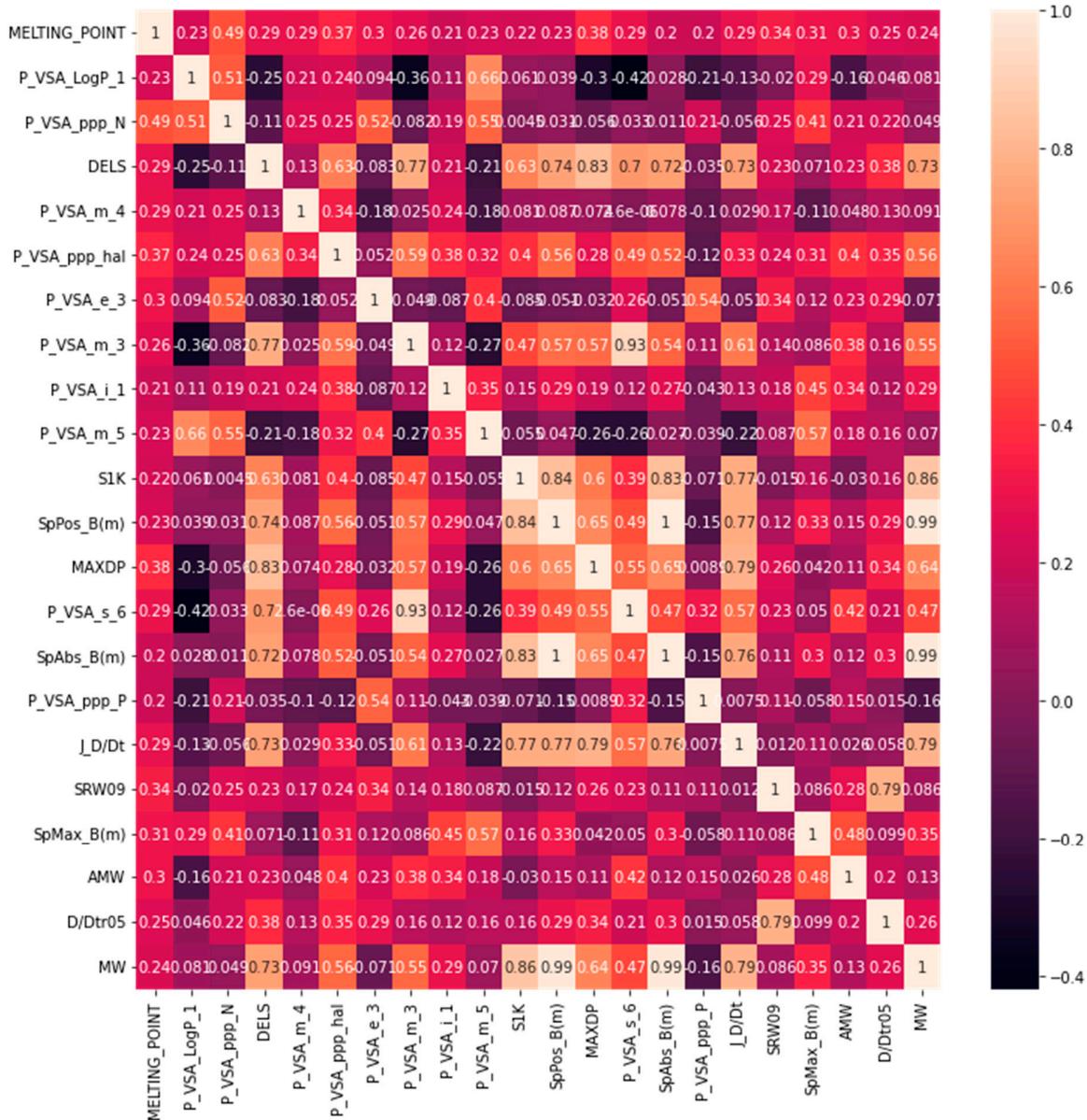


Figure S2. A correlation matrix comparing the melting point (T_m) with top 20 important molecular descriptors based on the Pearson correlation method. The numbers found in the correlation matrix is the feature correlation coefficients or ranking scores computed based on Pearson correlation method.

Table S2. The top 20 most important molecular descriptors obtained from DL-model based on 3 different correlation methods, i.e. Pearson, Spearman and Kendall.

Pearson	Spearman	Kendall
P_VSA_logP_1	DELS	P_VSA_ppp_hal
P_VSA_ppp_N	MW	P_VSA_m_4

DELS	P_VSA_logP_1	P_VSA_ppp_N
P_VSA_m_4	P_VSA_ppp_N	P_VSA_e_4
P_VSA_ppp_hal	MAXDP	DELS
P_VSA_e_3	P_VSA_m_4	P_VSA_e_3
P_VSA_m3	TPSA(Tot)	MW
P_VSA_i_1	P_VSA_ppp_hal	TIE
P_VSA_m_5	P_VSA_m_3	S2K
S1K	SsF	P_VSA_m_5
SpPos_B(m)	P_VSA_MR_3	TPSA(Tot)
MAXDP	P_VSA_p_2	SAacc
P_VSA_s_6	P_VSA_m5	P_VSA_s6
P_VSA_ppp_P	P_VSA_ppp_ter	SRW09
J_D/Dt	O%	T(O..O)
SRW09	P_VSA_ppp_A	P_VSA_i_1
SpMax_B(m)	P_VSA_e_3	X%
AMW	P_VSA_e_5	Chi_Dz(e)
D/Dtr05	J_Dz(m)	SsF

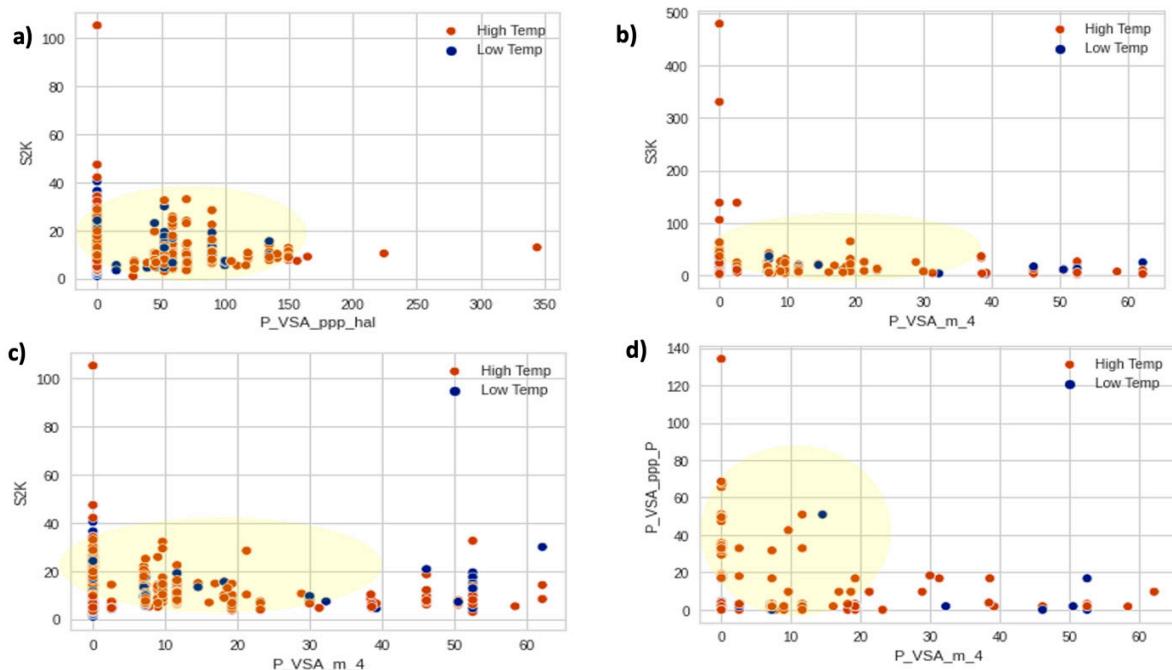


Figure S3. The distribution of the ILs melting points plot using the best combination of two molecular descriptors that mostly focus on the cations contribution: (a) S2K vs. $P_{VSA_ppp_hal}$; (b) S3K vs. P_{VSA_m} ; (c) S2K vs. $P_{VSA_m_4}$; (d) $P_{VSA_ppp_P}$ vs. $P_{VSA_m_4}$. The color of data points indicates the low melting point (i.e. $T_m < 273$ K) (in blue color) and high melting point (i.e. $T_m > 273$ K) (in brown color) of the corresponding ILs. The yellow region highlights the high melting point regime.