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Multicomponent ionic liquid CMC prediction

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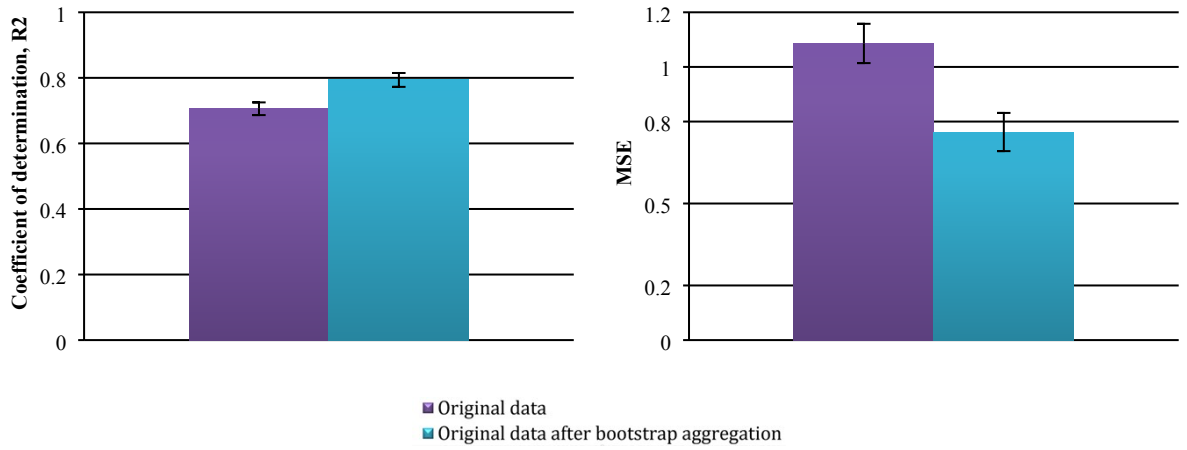

Figure S1. Comparison of different parameters describing the models created based on data before and after using bootstrap aggregation. Mean values of coefficient of determination R^2 and mean squared error MSE are presented with CI for 95% confidence level.

Table S1 Equation for ILs CMC predictions obtained with EA for 10 randomized sets of data after bootstrap aggregation after 150,000 generations

Set no	EA Equation	Complexity	R^2	MSE	Δ_{max}
1	lnCMC = 12.096145398611 + 0.0253961788407809×V_{ma} + 0.0134402271843192×C_s + 1.07706540507924×10^{-5}×V_m^2 - 0.0281722597929965×$\hat{S}$ - 4.09261980859347×10^{-5}×$\hat{S}$×C_s - 1.3650902159497×10^{-7}×V_{ma}×$\hat{S}^2$	33	0.803	0.754	2.87
2	lnCMC = 12.2969459736987 + 0.0129431313773733×C_s + 1.11567915379697×10-5×V_m^2 - 0.0288083398243091×$\hat{S}$ - 3.98208519964344×10-5×$\hat{S}$×C_s - 0.000127372885037649× $\Delta_{solv}G^{\infty}$×V_{ma} - 0.00014272436109066 5×V_m×V_{ma}	33	0.763	0.732	2.78
3	lnCMC = 9.63808068796259 + 0.0269828709349637×V_{ma} + 0.0166155637426254×C_s + 0.0148383827091835×V_m - 0.0325060528629139×$\hat{S}$ - 4.90518613041638×10^{-5}×$\hat{S}$×C_s - 1.46139585482021×10^{-7}×V_{ma}×$\hat{S}^2$	31	0.823	0.636	2.70
4	lnCMC = 9.84611806047204 + 0.0156121099436756×V_m + 0.0132986880733094×C_s - 0.0337652878658855×$\hat{S}$ - 4.06097753552024×10^{-5}×$\hat{S}$×C_s - 0.00012870009095876× $\Delta_{solv}G^{\infty}$×V_{ma} - 0.00014440387601042 8×V_m×V_{ma}	31	0.824	0.718	3.50
5	lnCMC = 13.8615906903276 + 3.82415481318421×10-5×C_s×T + 1.29337434225376×10^{-5}×V_m^2 - 0.00517784690723969×V_{ma} - 0.0331272566054945×$\hat{S}$ - 3.67954872762998×10^{-5}×$\hat{S}$×C_s	27	0.747	0.900	3.26
6	lnCMC = 12.1746586264027 + 0.0130352672329843×C_s + 0.000127204715304666×V_m×V_{ma} + 1.08788914528768×10^{-5}×V_m^2 - 0.0284828273827183×$\hat{S}$ - 3.98159712553106×10^{-5}×$\hat{S}$×C_s - 2.86981385815833×10^{-7}×V_{ma}×$\hat{S}^2$	35	0.776	0.763	2.81
7	lnCMC = 12.3636488059993 + 0.0123419518249543×C_s + 1.15355814674637×10^{-5}×V_m^2 - 0.0291746674073 72×$\hat{S}$ - 3.77910958255656×10-5×$\hat{S}$×C_s - 0.000133750490522388× $\Delta_{solv}G^{\infty}$×V_{ma} - 0.00014186455621749 02×V_m×V_{ma}	33	0.769	0.669	2.82
8	lnCMC = 12.3587764466037 + 3.45716604439926×10^{-5}×V_m×C_s + 1.12403710262679×10^{-5}×V_m^2 - 0.0289885330218974×$\hat{S}$ - 0.000129115378965499× $\Delta_{solv}G^{\infty}$×V_{ma} - 0.00014421339319152 9×V_m×V_{ma} - 1.01488616104132×10^{-7}×C_s×$\hat{S}^2$	37	0.837	0.694	2.98
9	lnCMC = 11.9129350547837 + 0.0473138453271865×V_{ma} + 0.0145318540796671×C_s + 9.37745733893398×10^{-6}×V_m^2 - 0.0270980870435032×$\hat{S}$ - 4.38140963933787×10^{-5}×$\hat{S}$×C_s - 0.000113398413450689×$\hat{S}$×V_{ma}	31	0.796	0.948	3.09
10	lnCMC = 12.3157953465308 + 0.0234920468134173×V_{ma} + 0.0137641637475242×C_s + 1.13182186803265×10^{-5}×V_m^2 - 0.0289437970384747×$\hat{S}$ - 4.17061347488651×10^{-5}×$\hat{S}$×C_s - 1.29702416519283×10^{-7}×V_m×$\hat{S}$×V_{ma}	33	0.799	0.779	3.21