

Expanding the chemical space using a Chemical Reaction Knowledge Graph

Supplementary information

Table S1. Search space for the hyperparameter optimization.

Hyperparameter	Range / Set
Number of Hops	{1, 2}
Sortpool k	[1, 1000]
Hidden Channels	{4, 8, 16, 32, 64, 128, 256, 512}
Number of Layers	[1, 12]
Learning Rate	{0.00001, 0.00005, 0.0001, 0.0005, 0.001, 0.01}
Dropout	[0.0, 0.99]
Decay	[0.0, 0.99]

Table S2. Result from the three rounds of the hyperparameter optimization.

Hyperparameter	Optimal Value
Validation AUC	0.89
Decay	0.85
Dropout	0.52
Number of Hidden channels	128
Learning rate	0.0005
Number of Hops	1
Number of Layers	6
Sortpool k	879