

Description of Additional Supplementary Files

File name: Supplementary Data 1

Description: The R^2 values on the prediction for unseen reactions by different methods

File name: Supplementary Data 2

Description: Performance of RS-coreset on the HTE datasets.

File name: Supplementary Data 3

Description: Performance of the B-H+ experiment.

File name: Supplementary Data 4

Description: Results of Lewis base-boryl radicals enabled coupling reaction.