

Description of Additional Supplementary Files

File Name: Supplementary Datasets 1-6

Description: Building Block Structures

File Name: Supplementary Dataset 7

Description: Building Block List

File Name: Supplementary Dataset 8

Description: Virtual Building Blocks with Predicted RRVs

File Name: Supplementary Dataset 9

Description: Experimental and Calculated Chemical Shifts

File Name: Supplementary Dataset 10

Description: Feature Selection Performance by 10-fold CV

File Name: Supplementary Dataset 11

Description: Performance of RRV Prediction by LOOCV

File Name: Supplementary Dataset 12

Description: Feature Selection for the Final RRV Predictor

File Name: Supplementary Dataset 13

Description: Rules in the Search Algorithm

File Name: Supplementary Dataset 14

Description: Tanimoto Similarity Matrix