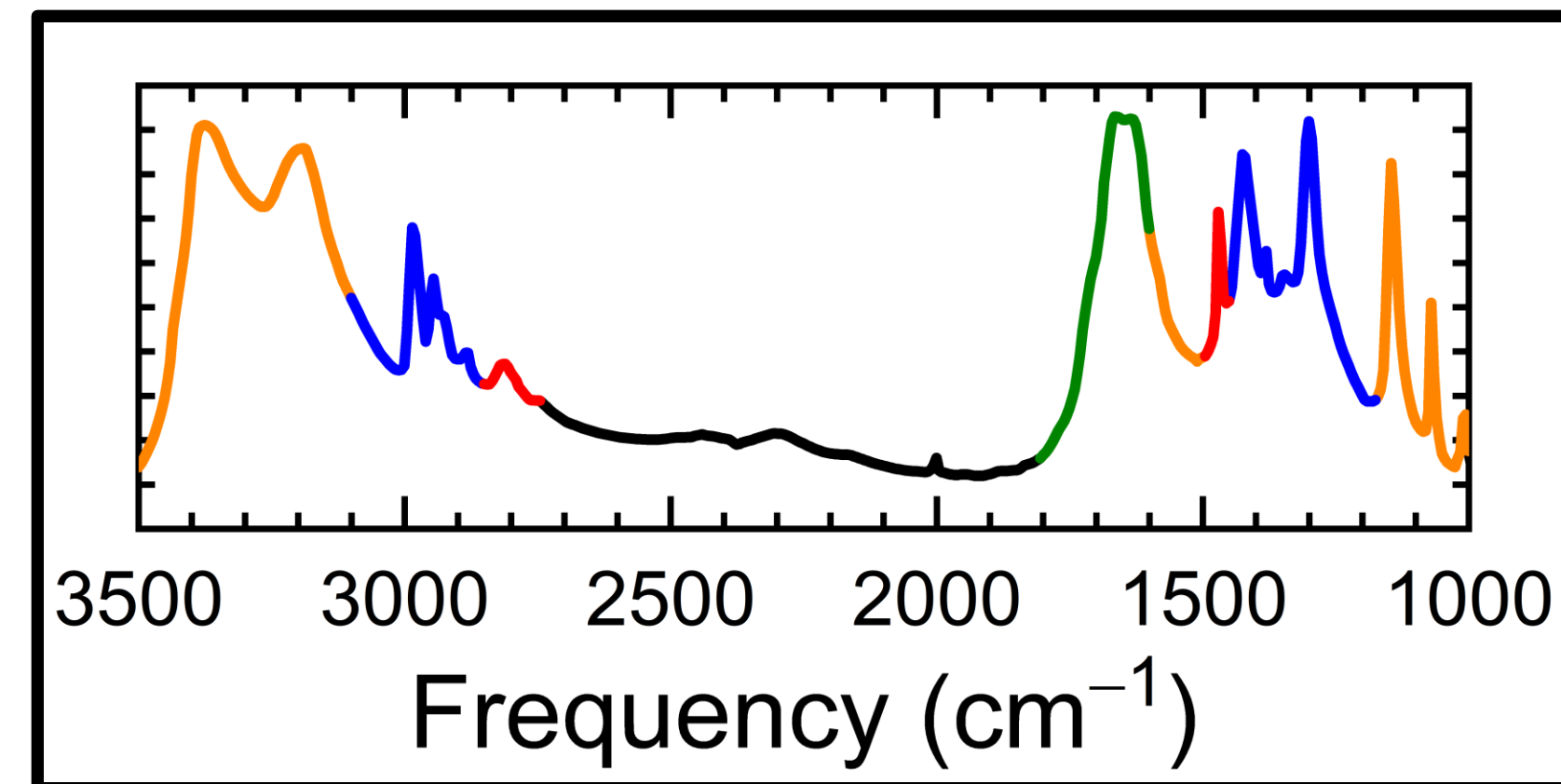


infrared spectrum

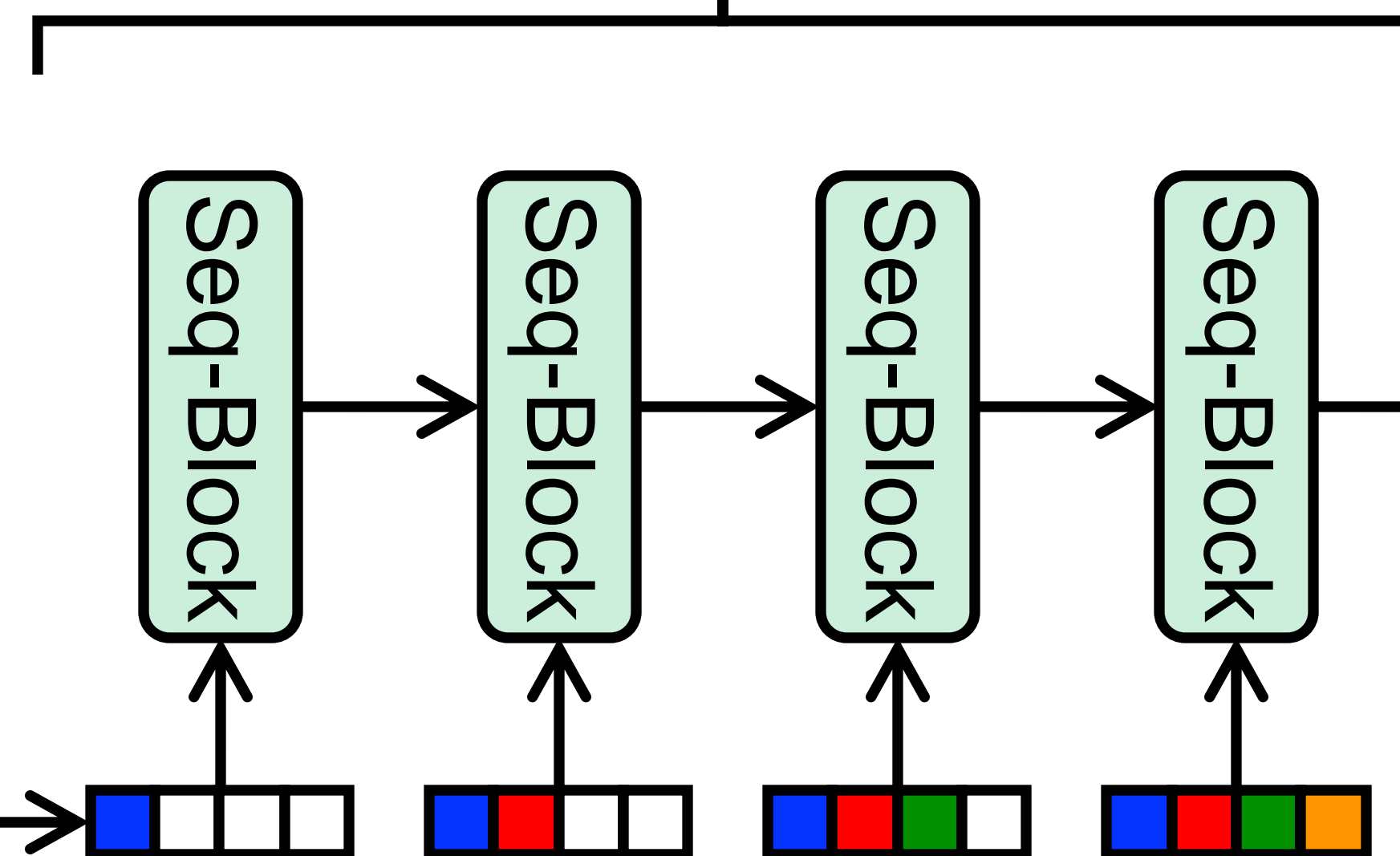


preprocess

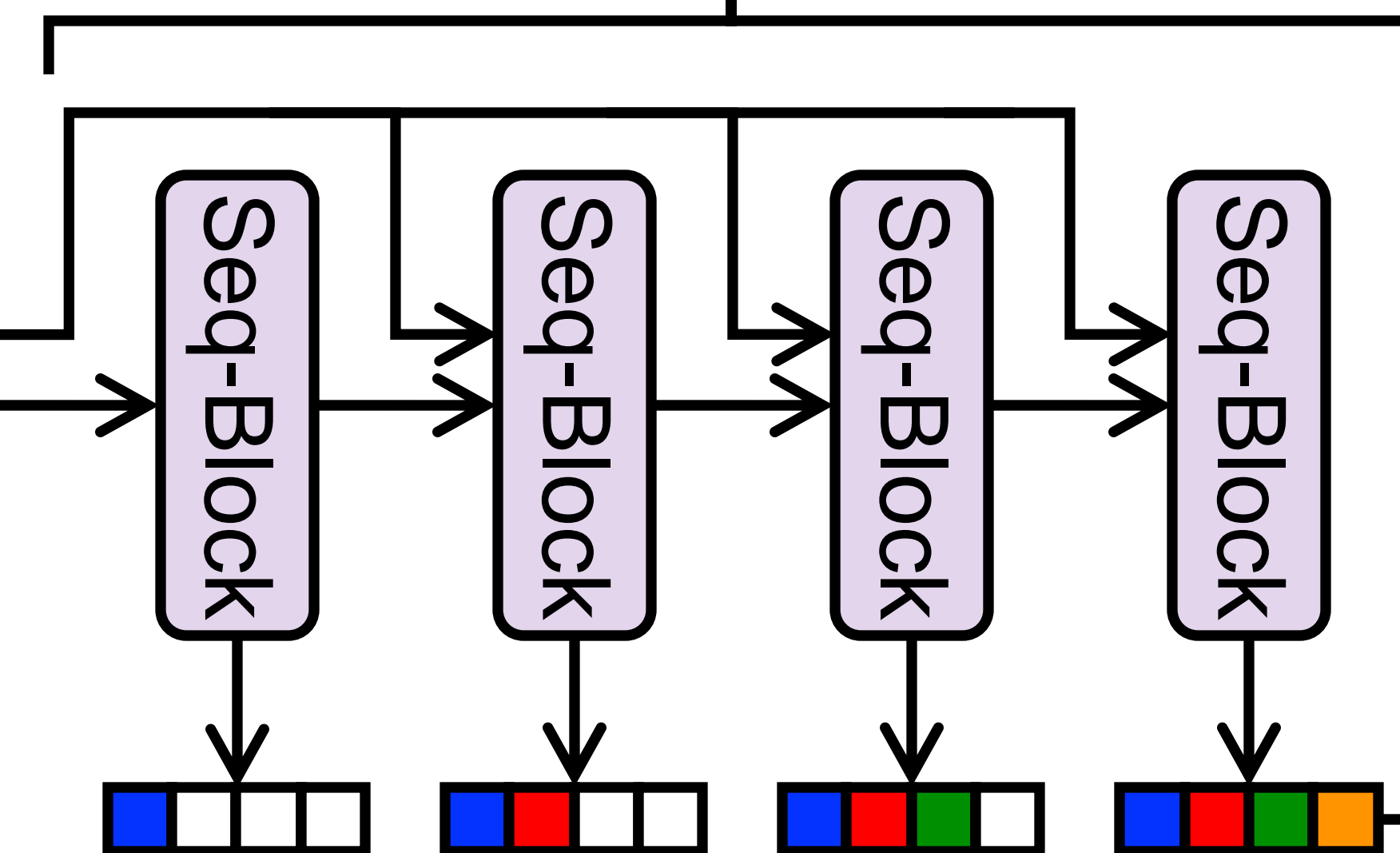
3366 83 3189 68 2978 43 2967 19  
 2942 34 2924 21 2880 19 2811 84  
 1662 96 1454 55 1420 71 1378 42  
 1298 56 1143 43 1068 26 1008 16

frequency-intensity pairs

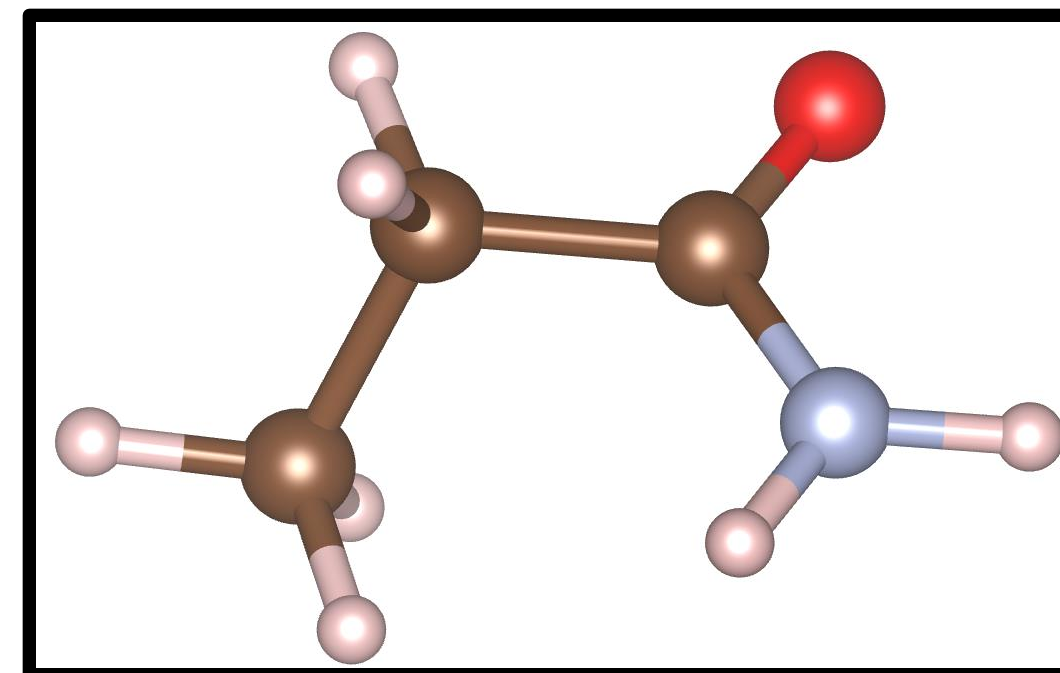
encoder



decoder



molecular structure



postprocess

[C][C][C][=Branch1  
 ][=O][N]CH<sub>3</sub>CH<sub>2</sub>C(  
 =O)NH<sub>2</sub>

SELFIES fingerprint