Supporting Information

RadicalRetro: A Deep Learning-Based Retrosynthesis Model for Radical Reactions

Jiangcheng Xu[1,2,*], Jun Dong[1,2], Kui Du[3], WenWen Liu[1,2], Jiehai Peng[4], Wenbo Yu[1,2,*]

1. Hangzhou Vocational & Technical College, Hangzhou, 310014, P. R. China

2. Hangzhou Engineering Research Center for Key Technology Improvement and Application of Novel Bio-based Materials, Hangzhou, 310014, P. R. China

3. School of Chemistry and Chemical Engineering, Shaoxing University, Shaoxing 312000, P. R. China

4. Zhejiang Medicine Co., Ltd., Hangzhou, 310014, P. R. China

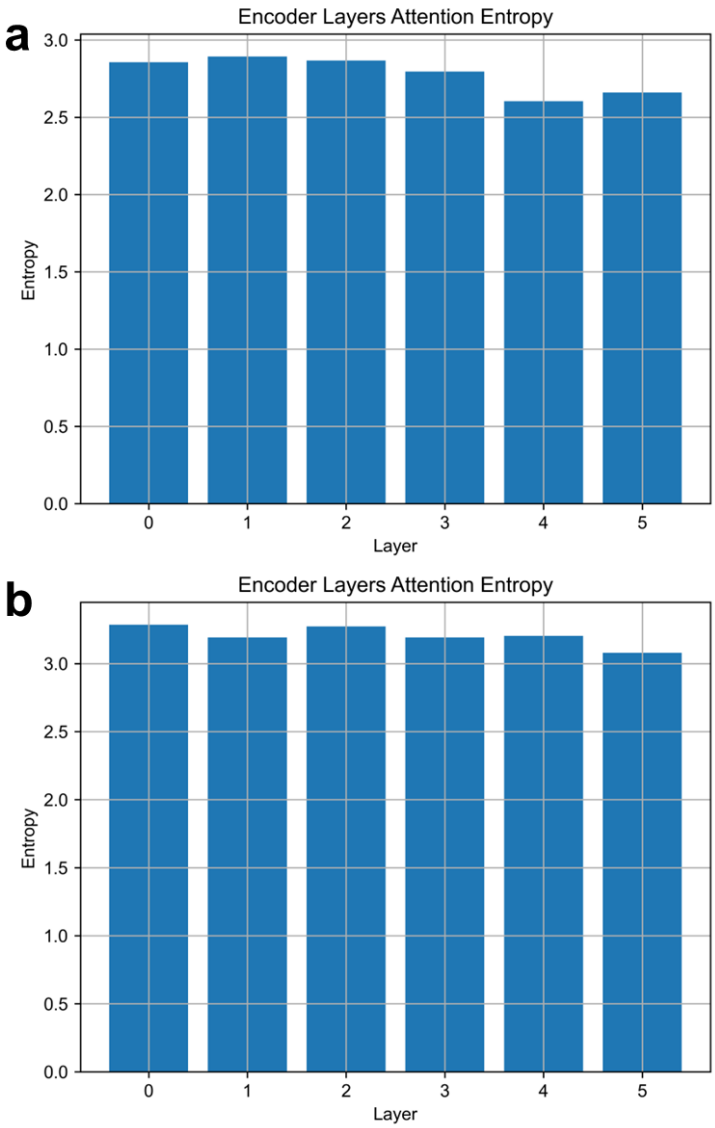


Figure S1. Attention Entropy Maps for Retrosynthetic Analysis of (a) 2-(2-phenyl-1H-indol-1-yl)acetonitrile and (b) Azapolycyclic Aromatic Hydrocarbons (PAHs). We calculated the attention entropy across all encoder layers for a representative sample and observed a gradual decline from the lower to higher layers (e.g., from 2.85 at Layer 0 to 2.65 at Layer 5). This trend suggests that the model's attention becomes more concentrated on specific tokens as depth increases. These findings support the interpretation that shallower layers capture broader contextual information, while deeper layers focus on chemically significant features such as reactive centers.

Attention Weight Heatmap for Retrosynthesis Prediction using RadicalRetro

Case 1:

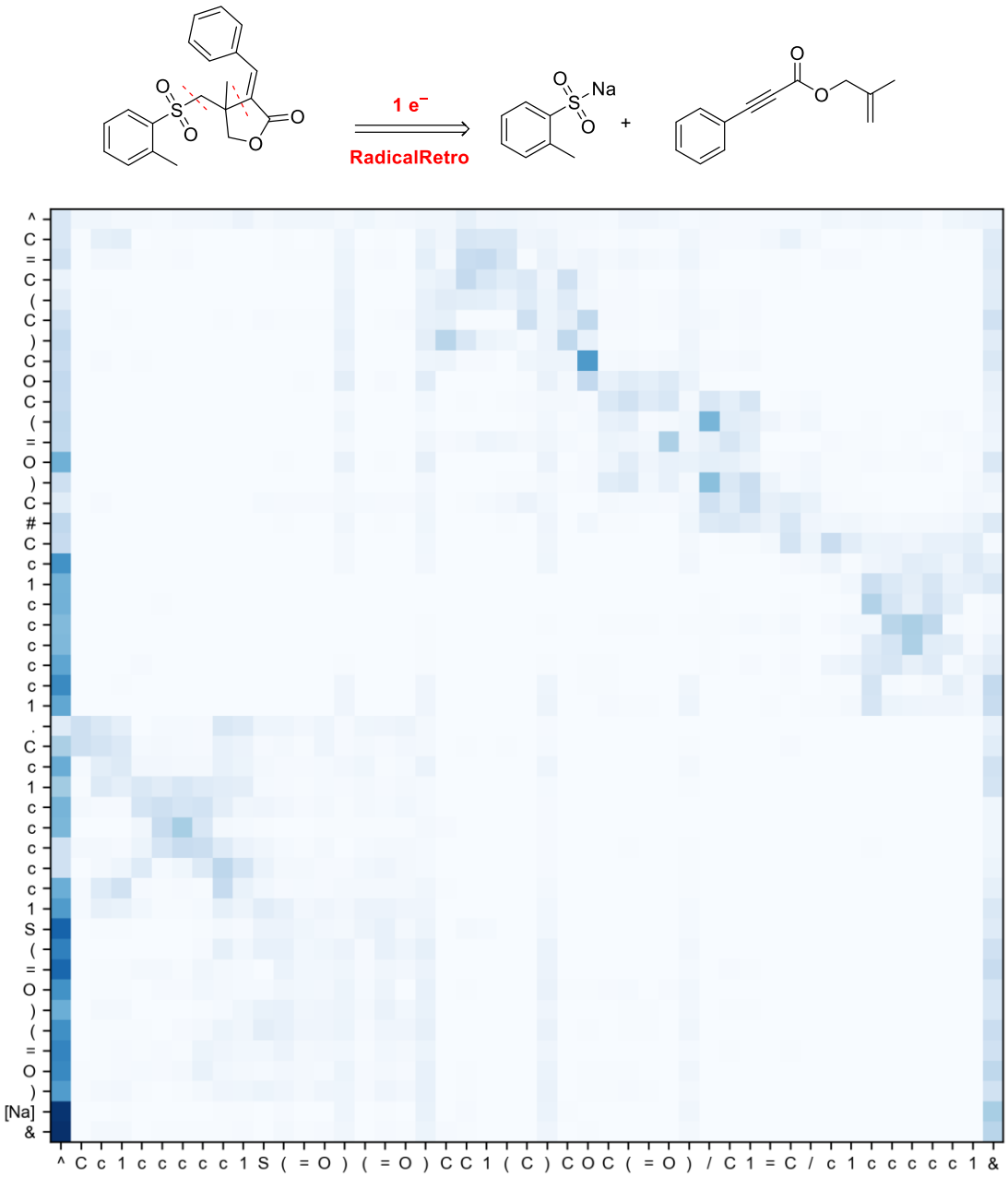


Figure S2 Case Study 1 of the RadicalRetro Retrosynthesis Attention Mechanism

Case 2:

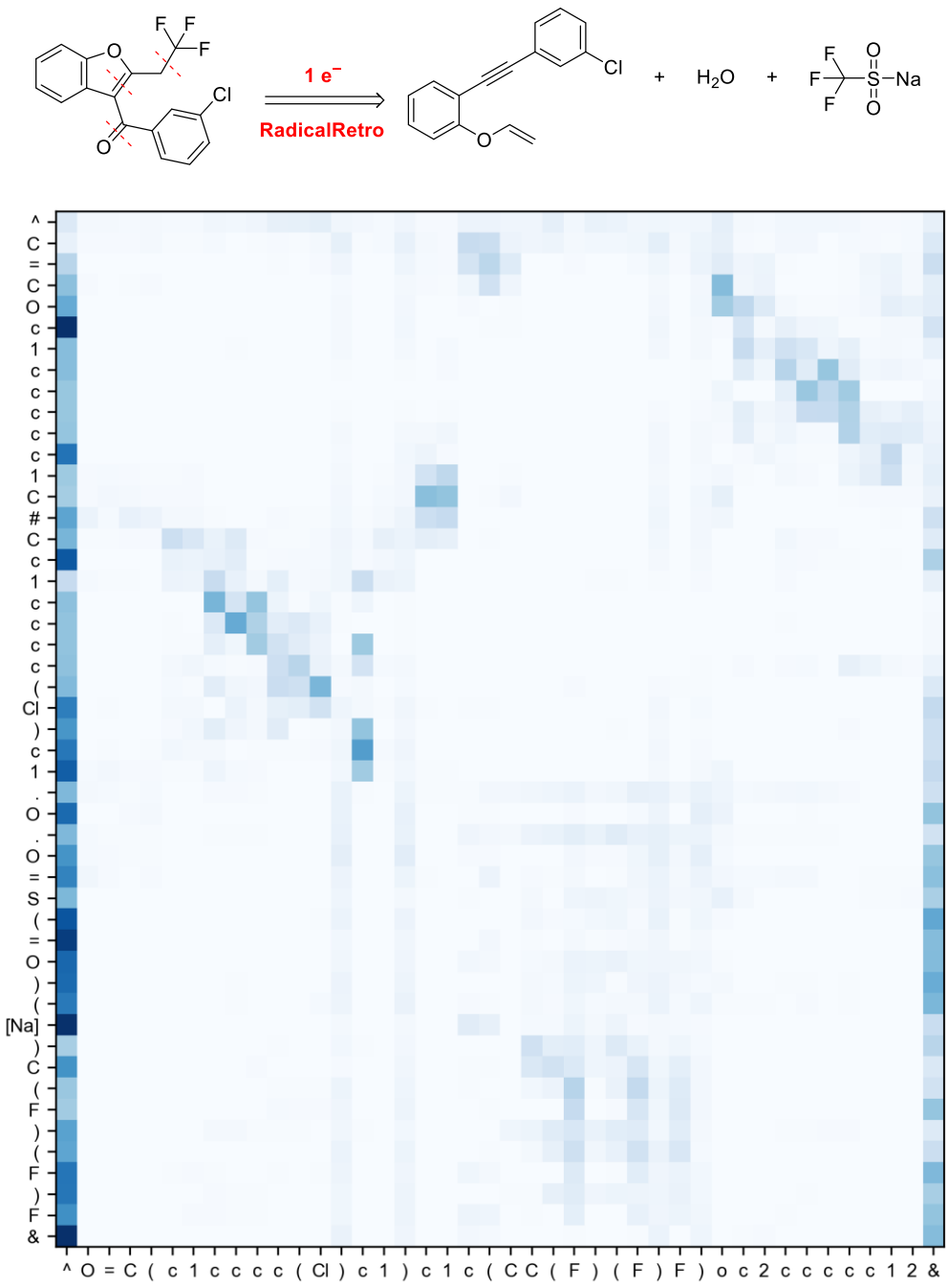
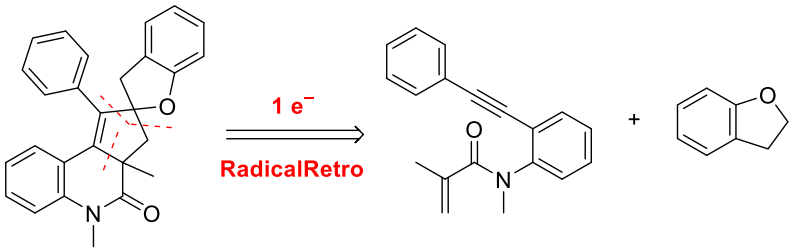


Figure S3 Case Study 2 of the RadicalRetro Retrosynthesis Attention Mechanism

Case 3:



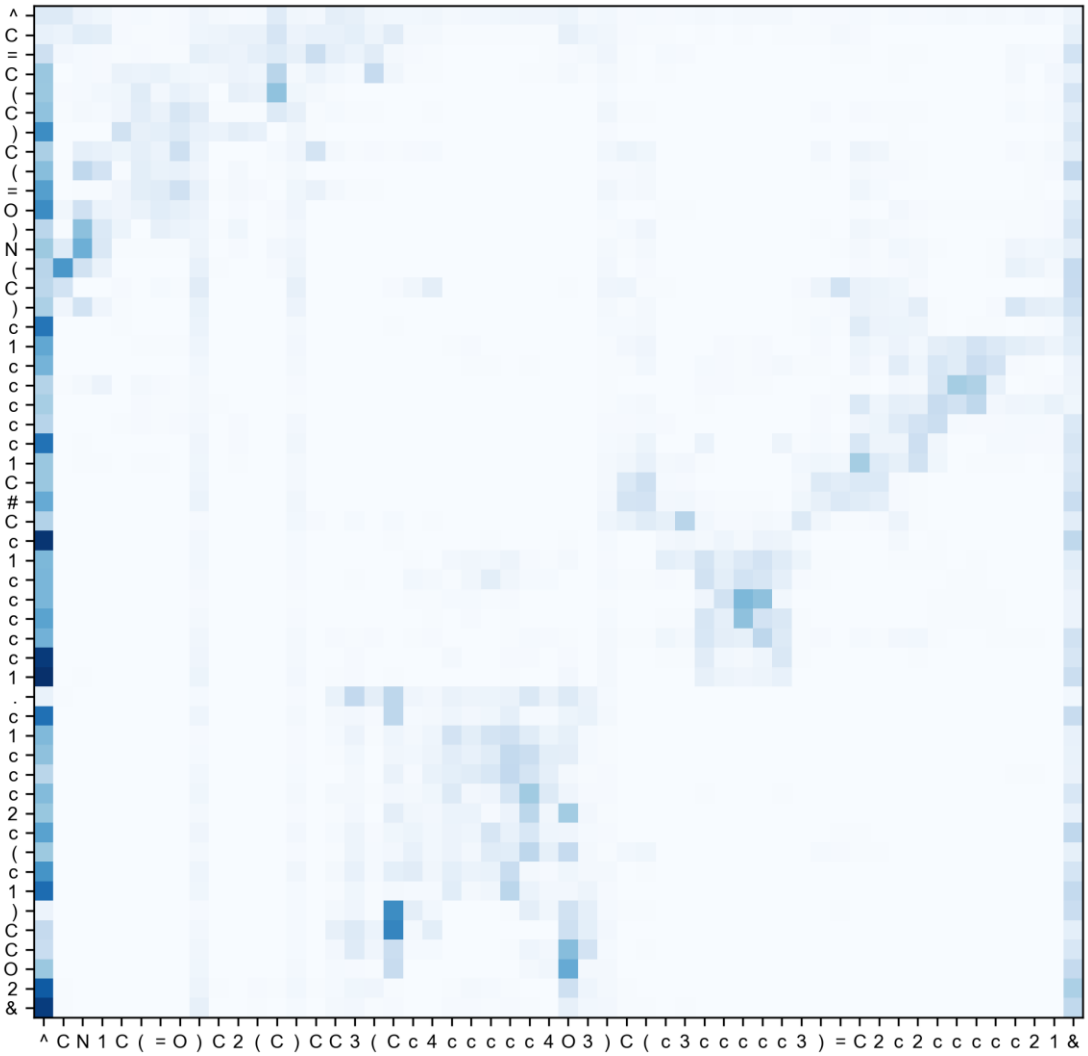


Figure S4. Case Study 3 of the RadicalRetro Retrosynthesis Attention Mechanism