

File Name: Supplementary Data 1.xlsx

Description: Computed iso-density and experimentally determined surfaces for each studied molecule

File Name: Supplementary Data 2

Description: xyz coordinates of all studied molecules

File Name: Source Data.xlsx

Description: Source data used in figures 1 and 2

File Name: Supplementary Software

Description: Scripts and sample input file for running Multiwfn code (Multiwfn.in), Orca code (orca_input.in), and Matlab code for computing molecular surfaces (analyze_surf.m)