We have uploaded the relevant calculation files to GitHub, organizing them by each small organic MALDI matrix. Within each matrix directory, subdirectories are further divided by different basis sets to facilitate user access and management. The calculation files follow the naming convention of “Functional-MALDI\_Matrix\_Abbreviation” (e.g., B3LYP-SA.log), clearly indicating the functional and matrix associated with each file. During the calculations, we used GaussView software to set parameters and generate input files (.gjf), which were then uploaded to a server for computation. The resulting output files (.log) contain detailed records of the computational parameters and results. With this clear directory structure and comprehensive calculation records, we aim to provide convenient support for research reproducibility and further exploration.