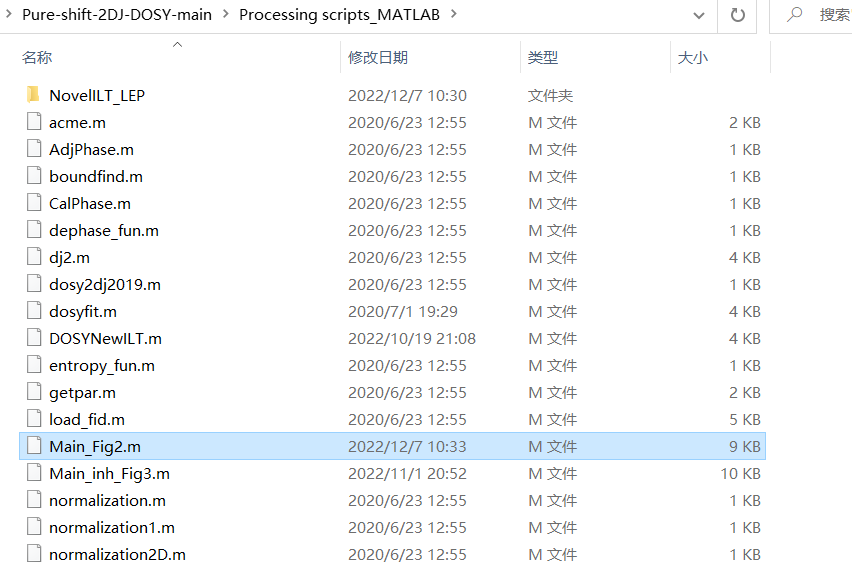
**The operation manual for data processing on Pure-shift 2D*J*-DOSY data**

***1. Download the full zip file from the GitHub site.***

***2. Unzip the master file named “Pure-shift-2DJ-DOSY-main”.***

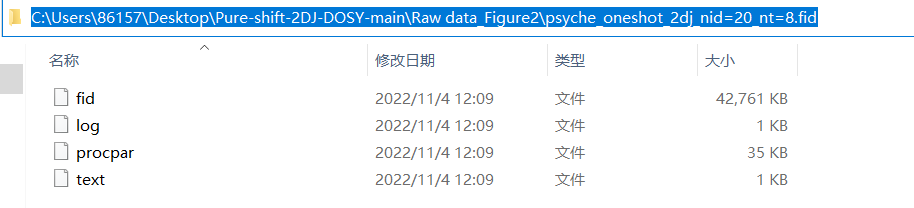
***3. Open the Matlab main function.***

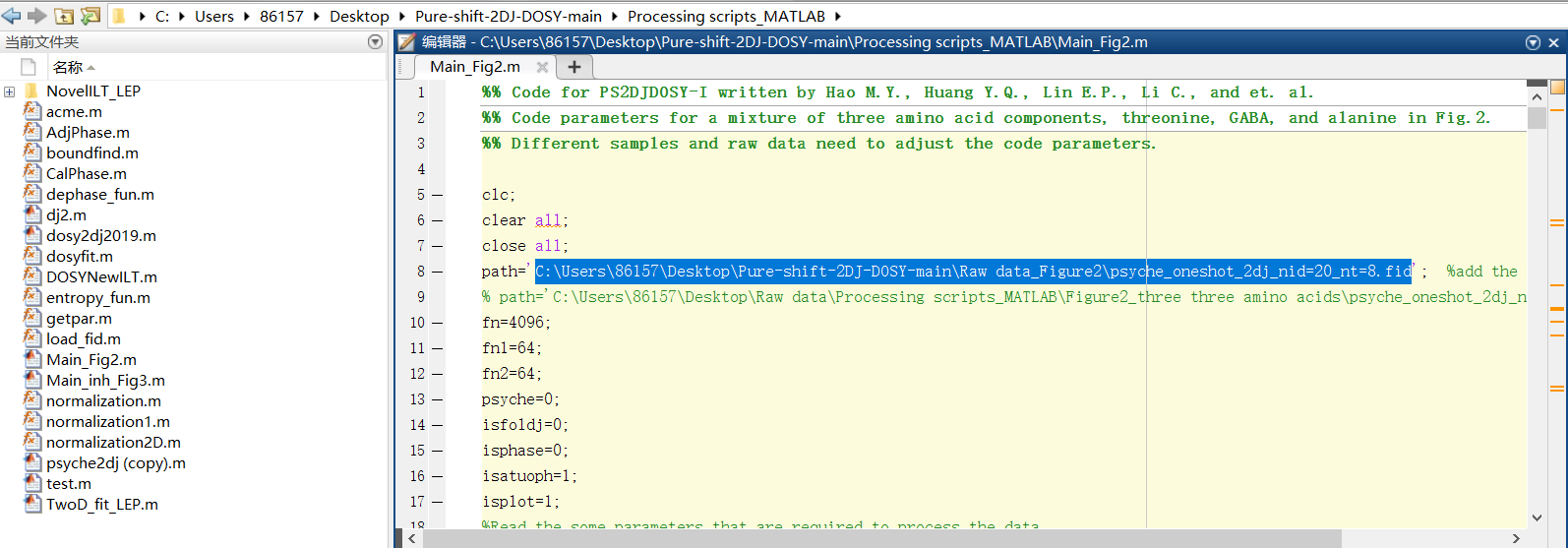
*For example, the main function named “Main\_Fig2” is used to process the pure shift 2DJ-DOSY data for three amino acid components, and to generate Figure 2 shown in the manuscript. Similarly, the main function named “Main\_inh\_Fig3” is adopted to generate Figure 3 shown in the manuscript. It should be noted that the code parameters need to be well adjusted for different samples and raw data.*



***4. Copy and paste the right path of the raw data into the main function script.***

*Copy the path of the raw data and paste it into the main function script as shown following.*





***5. Run the main function.***

*Run the main function script to obtain the resulting spectra. For Figures 2 and 3, the suitable parameters have been set in the main functions “Main\_Fig2” and “Main\_Fig3”, respectively, and they can be directly run to obtain the resulting spectra.*

