pSimulate user guide v1

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Compile pSimulate

1. Download MinGW and MSYS
2. Set the paths of MINGW_HOME and MSYS_HOME
3. Goto the folder of pSimulate, and type make.bat kernel in cmd
4. Once the compile is done, the executable program is located in installer/pSimulate

Generate simulated spectra

1. Goto the installer/pSimulate folder
2. Customize the parameter file in example folder
3. Goto the bin folder, and type pSimulate.exe bs3.cfg, where the bs3.cfg is the parameter file used to generate bs3 cross-linked spectra, you change it to ss.cfg in example folder
4. Find the simulated dataset in result_output_path which was set in the bs3.cfg