This section provides initial values and bound conditions for the fitting, as shown in Table SⅠ.

TABLE SI

INITIAL VALUES AND BOUNDARY CONDITIONS FOR MULTIPOOL LORENTZIAN FITTING

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  |  | | **Amide** | | **MT** | **DS** | **NOE** | **Creatine** |
| **Amplitude** | | up | | 0.3 | 0.5 | 1 | 0.3 | 0.2 |
| iv | | 0.02 | 0.1 | 0.9 | 0.05 | 0.02 |
| lb | | 0.01 | 0.05 | 0.7 | 0.01 | 0.01 |
| **FWHM** | | up | | 5 | 150 | 5 | 25 | 2 |
| iv | | 1.25 | 10 | 1.25 | 1.5 | 1 |
| lb | | 2 | 15 | 2.5 | 3.0 | 1 |
| **Frequency**  **offset** | | up | | 3.8 | -1.5 | 1 | -3.3 | 2.2 |
| iv | | 3.5 | -2 | 0 | -3.5 | 2 |
| lb | | 3.2 | -2.2 | -1 | -3.7 | 1.6 |