

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

TABLE SI

INITIAL VALUES AND BOUNDARY CONDITIONS FOR MULTIPOL 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