

Supplementary table S2: Metabolite concentration ratios to total Creatine

| | Control (n=12) | | Case (n=9) | | Treated (n=9) | |
|---------------|----------------|------|------------|------|---------------|------|
| | Mean | SD | Mean | SD | Mean | SD |
| tCho | 0.36 | 0.05 | 0.35 | 0.06 | 0.33 | 0.06 |
| %CRLB | 4 | 0.7 | 4.4 | 0.9 | 3.3 | 0.5 |
| tNAA | 1.21 | 0.17 | 1.21 | 0.11 | 1.1 | 0.14 |
| %CRLB | 4.4 | 0.7 | 4.3 | 1 | 3.9 | 0.8 |
| mI+Gly | 1.18 | 0.11 | 1.11 | 0.11 | 1.17 | 0.1 |
| %CRLB | 4.8 | 0.9 | 5 | 1.2 | 3.8 | 1.1 |
| NAA | 1.02 | 0.13 | 1.01 | 0.17 | 0.91 | 0.07 |
| %CRLB | 5.2 | 0.8 | 5.6 | 1.4 | 5 | 1.1 |
| Glx | 1.78 | 0.22 | 1.81 | 0.15 | 1.57 | 0.21 |
| %CRLB | 7.6 | 1.1 | 7.3 | 1.1 | 7.1 | 1.6 |
| mI | 1.01 | 0.12 | 0.89 | 0.17 | 0.98 | 0.14 |
| %CRLB | 9.1 | 3.3 | 11.2 | 3.3 | 7.8 | 3.3 |
| Glu | 1.33 | 0.19 | 1.3 | 0.11 | 1.16 | 0.24 |
| %CRLB | 9.1 | 1.7 | 9.3 | 1.7 | 8.9 | 2.5 |
| Gln | 0.45 | 0.08 | 0.51 | 0.15 | 0.4 | 0.15 |
| %CRLB | 26.1 | 3.9 | 24 | 4.4 | 26.4 | 8.2 |

| | | | | | | |
|---------------|-------|-------|-------|-------|-------|-------|
| Asp | 0.46 | 0.13 | 0.48 | 0.12 | 0.44 | 0.09 |
| %CRLB | 29.2 | 15.2 | 25.9 | 9 | 24.2 | 7.5 |
| NAAG | 0.19 | 0.07 | 0.2 | 0.09 | 0.18 | 0.08 |
| %CRLB | 30.8 | 14.6 | 29.3 | 12.5 | 28.4 | 15.6 |
| GSH | 0.18 | 0.1 | 0.19 | 0.05 | 0.13 | 0.05 |
| %CRLB | 36.6 | 26.8 | 27.9 | 6.1 | 35.3 | 16.7 |
| GABA | 0.16 | 0.05 | 0.14 | 0.08 | 0.14 | 0.07 |
| %CRLB | 51.1 | 17.9 | 60.6 | 20.3 | 60 | 29.3 |
| Asc | 0.48 | 0.21 | 0.46 | 0.07 | 0.5 | 0.09 |
| %CRLB | 102.2 | 282.6 | 22.4 | 6 | 17.3 | 5.4 |
| Scyllo | 0.03 | 0.02 | 0.02 | 0.02 | 0.02 | 0.02 |
| %CRLB | 136.8 | 274 | 251.6 | 378.1 | 182.3 | 314 |
| Glc | 0.17 | 0.12 | 0.17 | 0.05 | 0.18 | 0.06 |
| %CRLB | 155.8 | 290.9 | 41.6 | 23.3 | 33.3 | 12.9 |
| PE | 0.32 | 0.25 | 0.19 | 0.1 | 0.24 | 0.13 |
| %CRLB | 160.4 | 301.2 | 173.8 | 312.2 | 151.3 | 319 |
| Gly | 0.17 | 0.16 | 0.22 | 0.12 | 0.2 | 0.14 |
| %CRLB | 246.8 | 364.7 | 58.1 | 32.9 | 165.9 | 323 |
| Lac | 0.09 | 0.1 | 0.03 | 0.04 | 0.06 | 0.06 |
| %CRLB | 453.2 | 482.1 | 565.8 | 421 | 316.2 | 393.6 |

| | | | | | | |
|--------------|-------|-------|-------|-------|-------|-------|
| Tau | 0.05 | 0.07 | 0.04 | 0.05 | 0.03 | 0.02 |
| %CRLB | 557.7 | 470.2 | 594 | 480.4 | 486.7 | 400.7 |
| Ala | 0.03 | 0.04 | 0.06 | 0.06 | 0.06 | 0.05 |
| %CRLB | 587.9 | 434.2 | 410.9 | 447.3 | 391.4 | 456.9 |

Legend: tCho: total choline; CRLB: Cramér Rao lower bounds; tNAA: total N-acetyl aspartate; mI: myoinositol; Gly: glycine; NAA: N-acetyl aspartate; Glx: glutamate-glutamine complex; Glu: glutamate; Gln: glutamine; Asp: aspartate; NAAG: N-acetylaspartyglutamate; GSH: glutathione; GABA: gamma-amino-butyrate; Asc: ascorbate; Scyllo: scyllo-inositol; Glc: glucose; PE: phosphoethanolamine; Lac: lactate; Tau: taurine; Ala: alanine.