

## NMR-based metabolomic analysis for the effects of alanyl-glutamine supplementation on C2C12 myoblasts injured by energy deprivation

Zhiqing Liu<sup>a</sup>, Caihua Huang<sup>b</sup>, Yan Liu<sup>a,\*</sup>, Donghai Lin<sup>a,\*</sup>, Yufen Zhao<sup>a</sup>

- <sup>a</sup> College of Chemistry and Chemical Engineering, Xiamen University, The Key Laboratory for Chemical Biology of Fujian Province, MOE Key Laboratory of Spectrochemical Analysis & Instrumentation, Xiamen 361005, China. E-mail: [dhlin@xmu.edu.cn](mailto:dhlin@xmu.edu.cn), Tel: +86-592-218-6078; [stacyliu@xmu.edu.cn](mailto:stacyliu@xmu.edu.cn), Tel: +86-592-218-5610.
- <sup>b</sup> Exercise and Health Laboratory, Xiamen University of Technology, Xiamen 361024, China

### Figure Legends

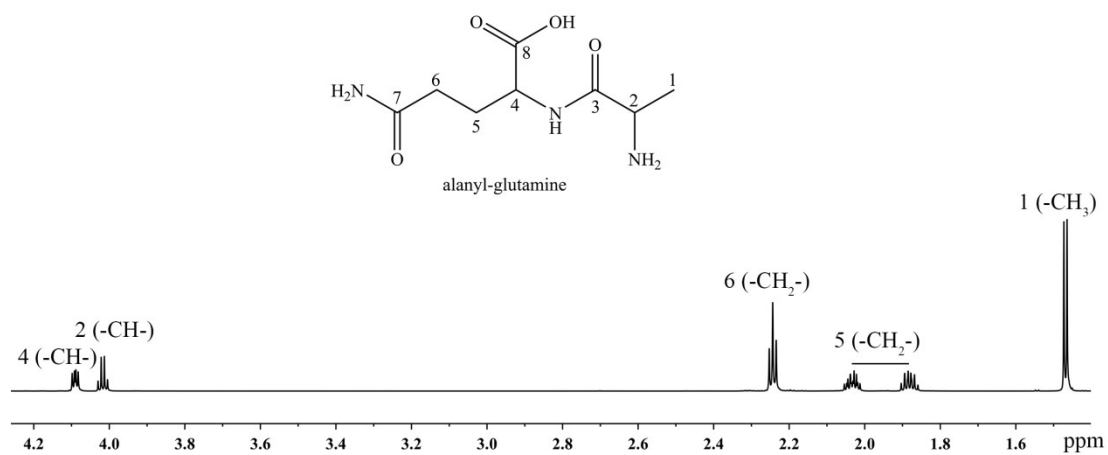
**Figure S1.** A representative 1D <sup>1</sup>H NMR spectrum of Ala-Gln dissolved in D<sub>2</sub>O recorded on 850 MHz NMR spectrometer at 298K.

**Figure S2.** A representative 2D <sup>1</sup>H-<sup>13</sup>C HSQC spectrum of aqueous extracts derived from C2C12 myoblast cells recorded on 850 MHz NMR spectrometer at 298K in PBS (pH 7.4).

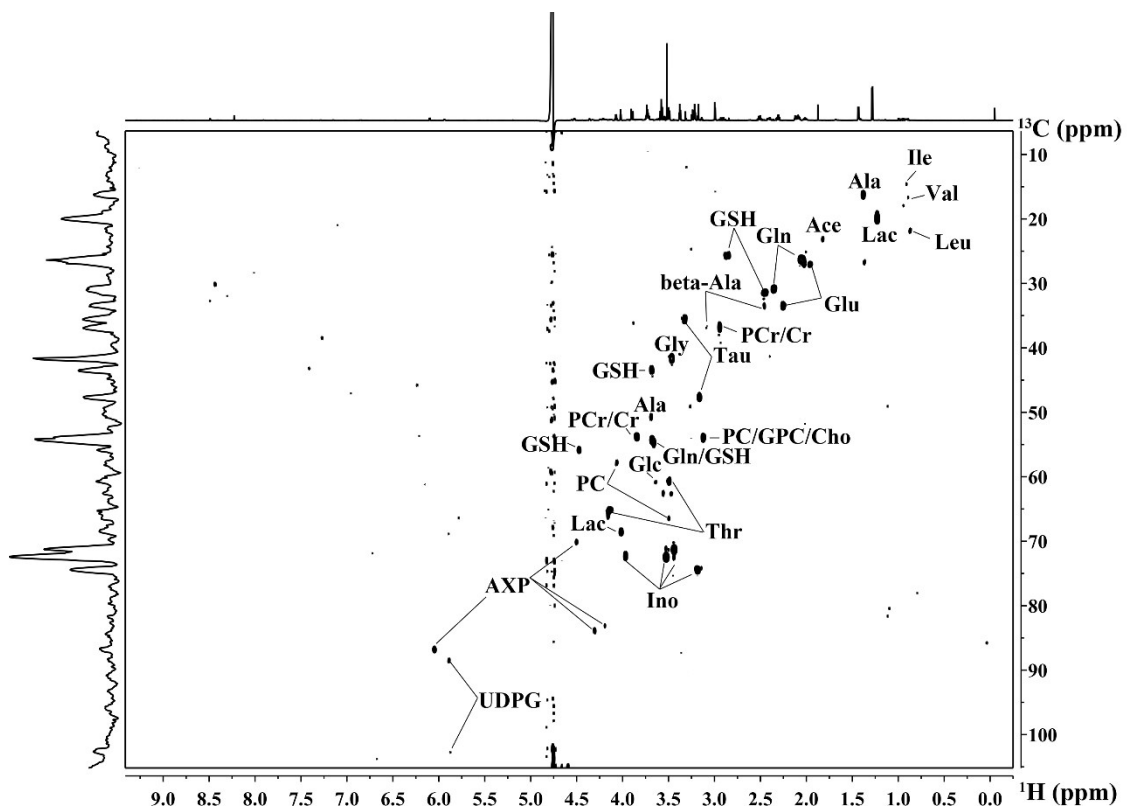
**Figure S3.** A selected region (0.8-2.8 ppm) of a representative 2D <sup>1</sup>H-<sup>1</sup>H TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.

**Figure S4.** A selected region (2.0-4.6 ppm) of a representative 2D <sup>1</sup>H-<sup>1</sup>H TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.

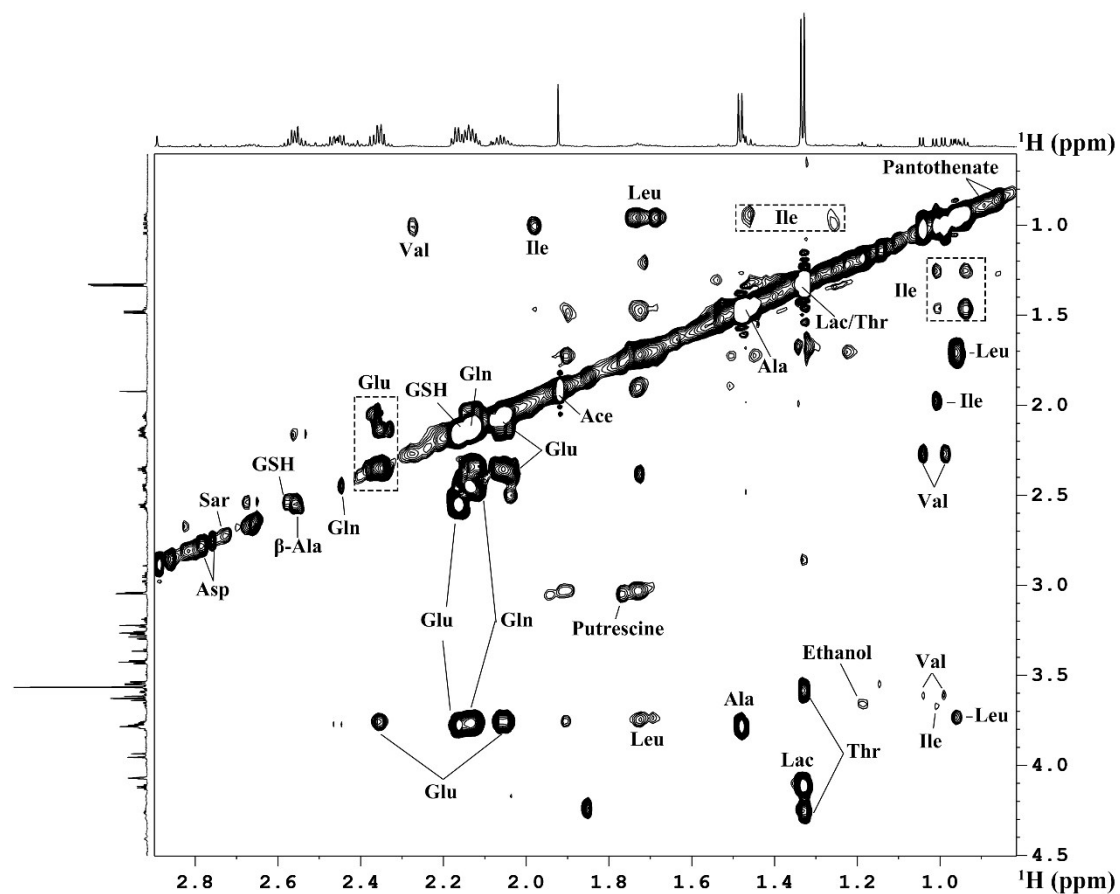
**Figure S5.** A selected region (5.5-9.5 ppm) of a representative 2D <sup>1</sup>H-<sup>1</sup>H TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.



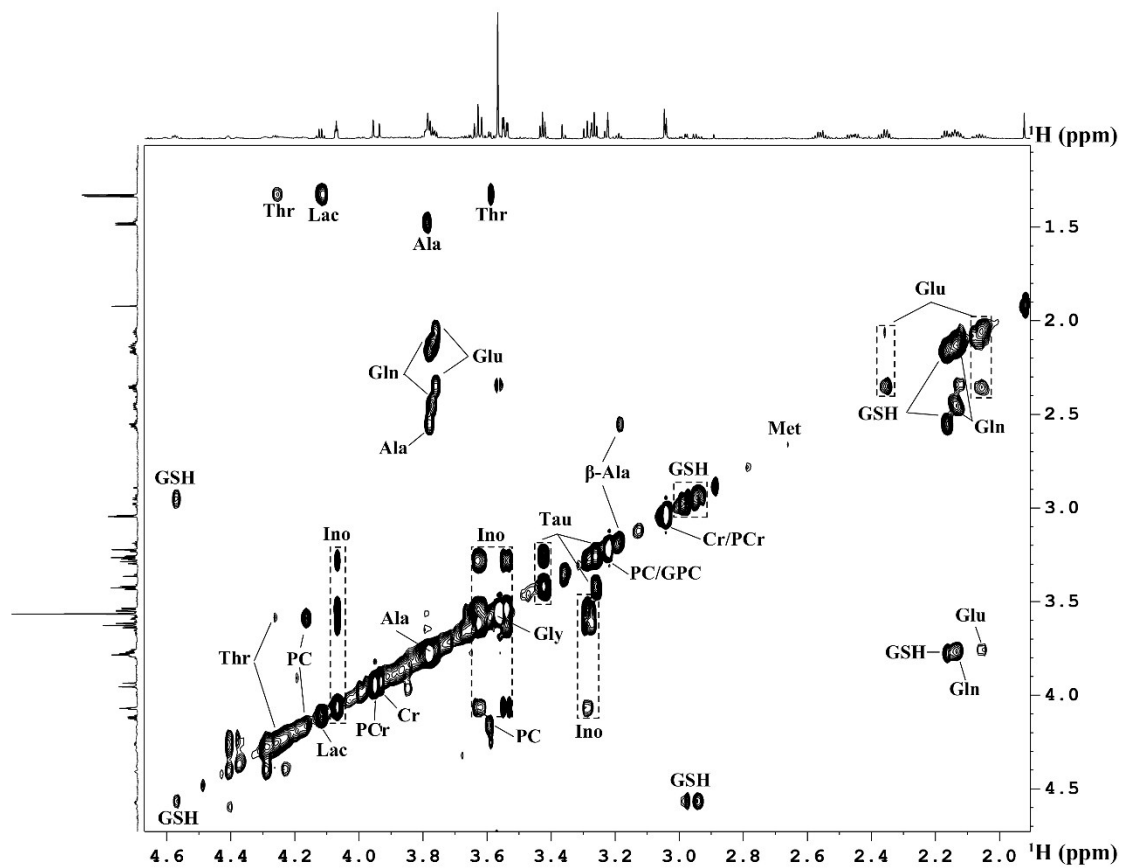
**Fig. S1** A representative 1D <sup>1</sup>H NMR spectrum of Ala-Gln dissolved in D<sub>2</sub>O recorded on 850 MHz NMR spectrometer at 298K.



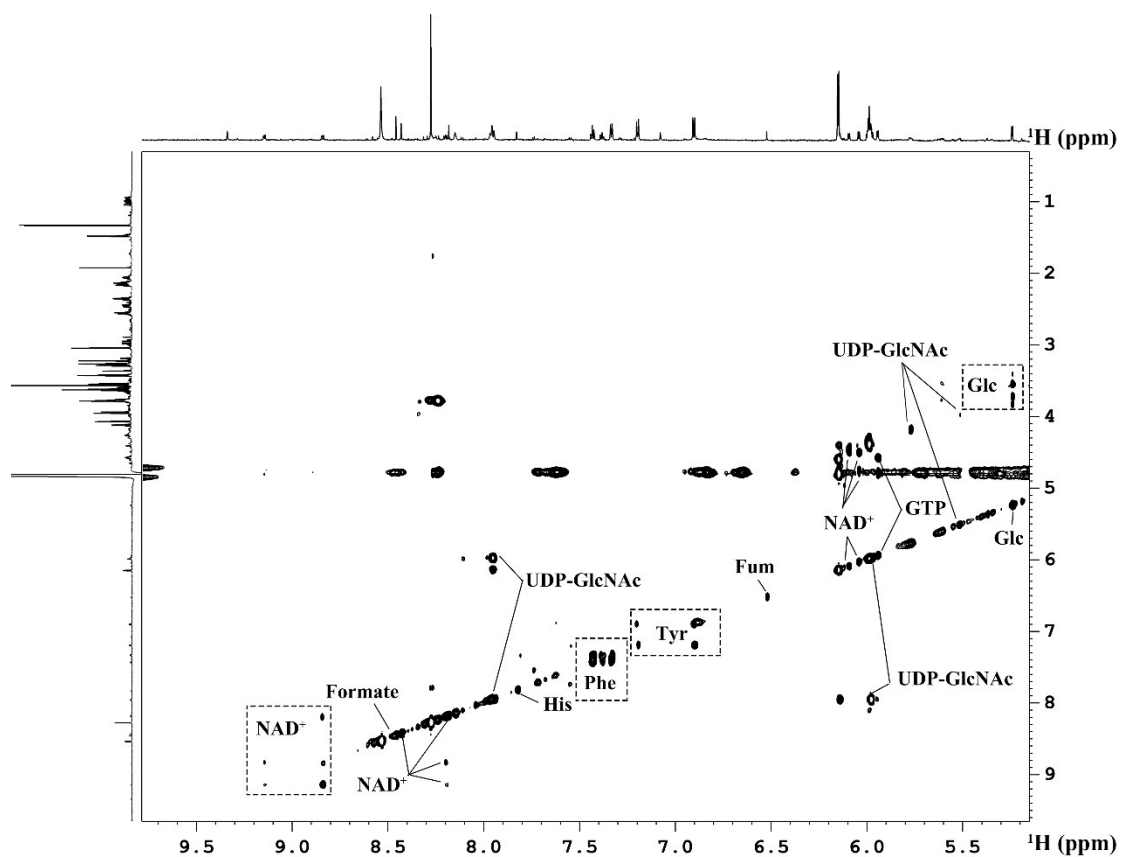
**Fig. S2** A representative 2D  $^1\text{H}$ - $^{13}\text{C}$  HSQC spectrum of aqueous extracts derived from C2C12 myoblast cells recorded on 850 MHz NMR spectrometer at 298K in PBS (pH 7.4).



**Fig. S3** A selected region (0.8-2.8 ppm) of a representative 2D  $^1\text{H}$ - $^1\text{H}$  TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.



**Fig. S4** A selected region (2.0-4.6 ppm) of a representative 2D  $^1\text{H}$ - $^1\text{H}$  TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.



**Fig. S5** A selected region (5.5-9.5 ppm) of a representative 2D  $^1\text{H}$ - $^1\text{H}$  TOCSY spectrum of aqueous extracts derived from C2C12 cells recorded at 298K in PBS (pH 7.4). Resonance assignments are labeled.