Electronic Supplementary Material (ESI) for Molecular Omics.

Supporting Information for

Proteomic and Metabolomic Profiling of Acute and Chronic Stress Events Associated with Military Exercises

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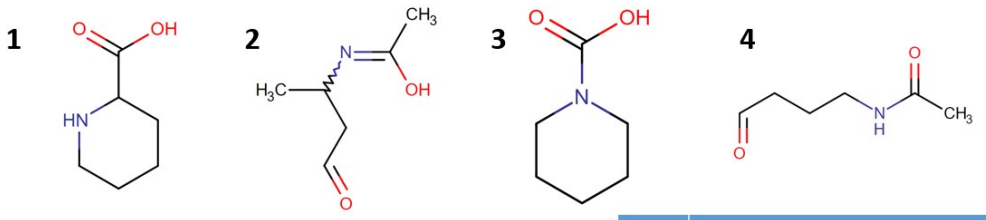
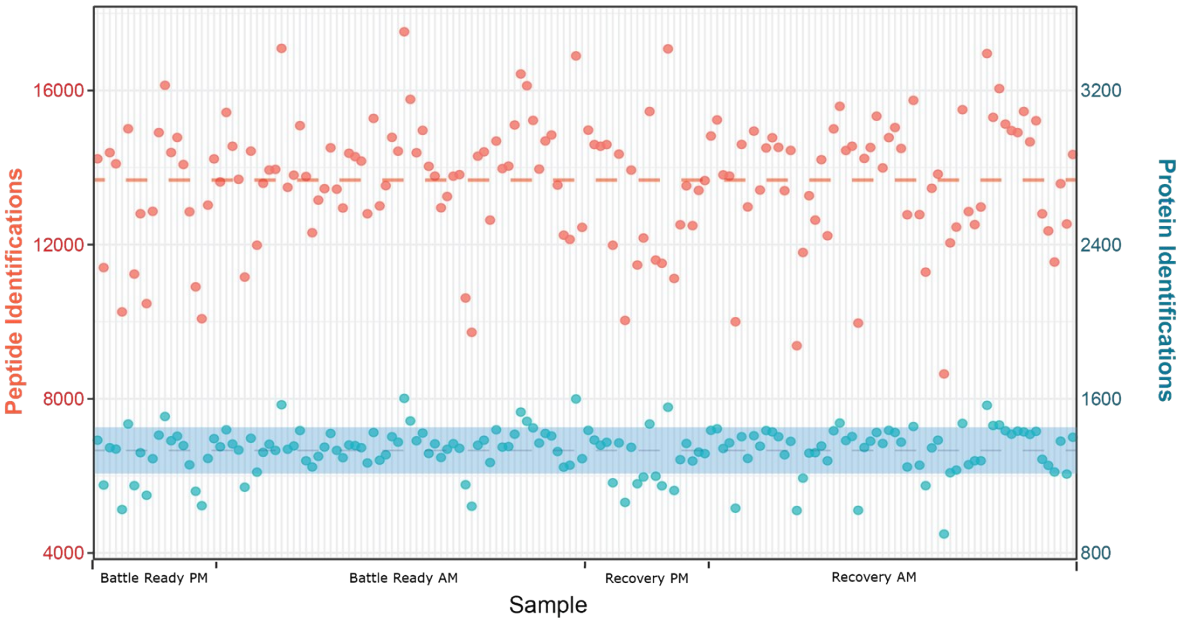
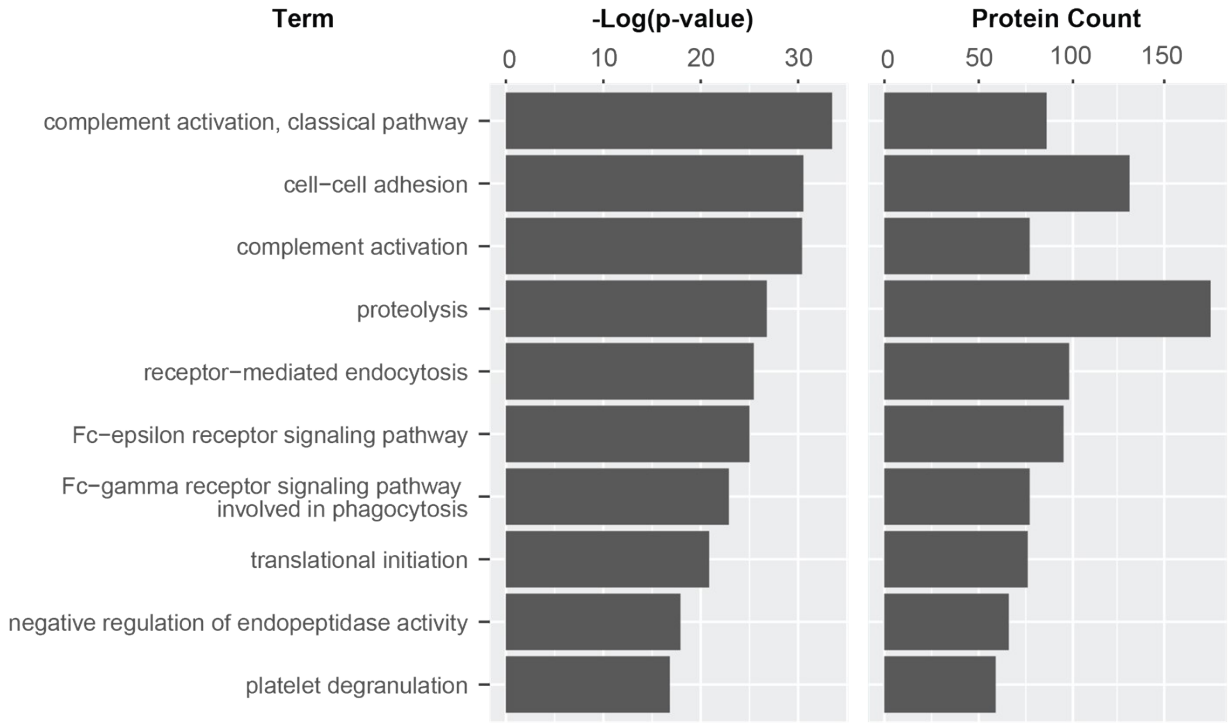
Supplemental Table 1: Potential identifications for pipecolic acid-like compounds.



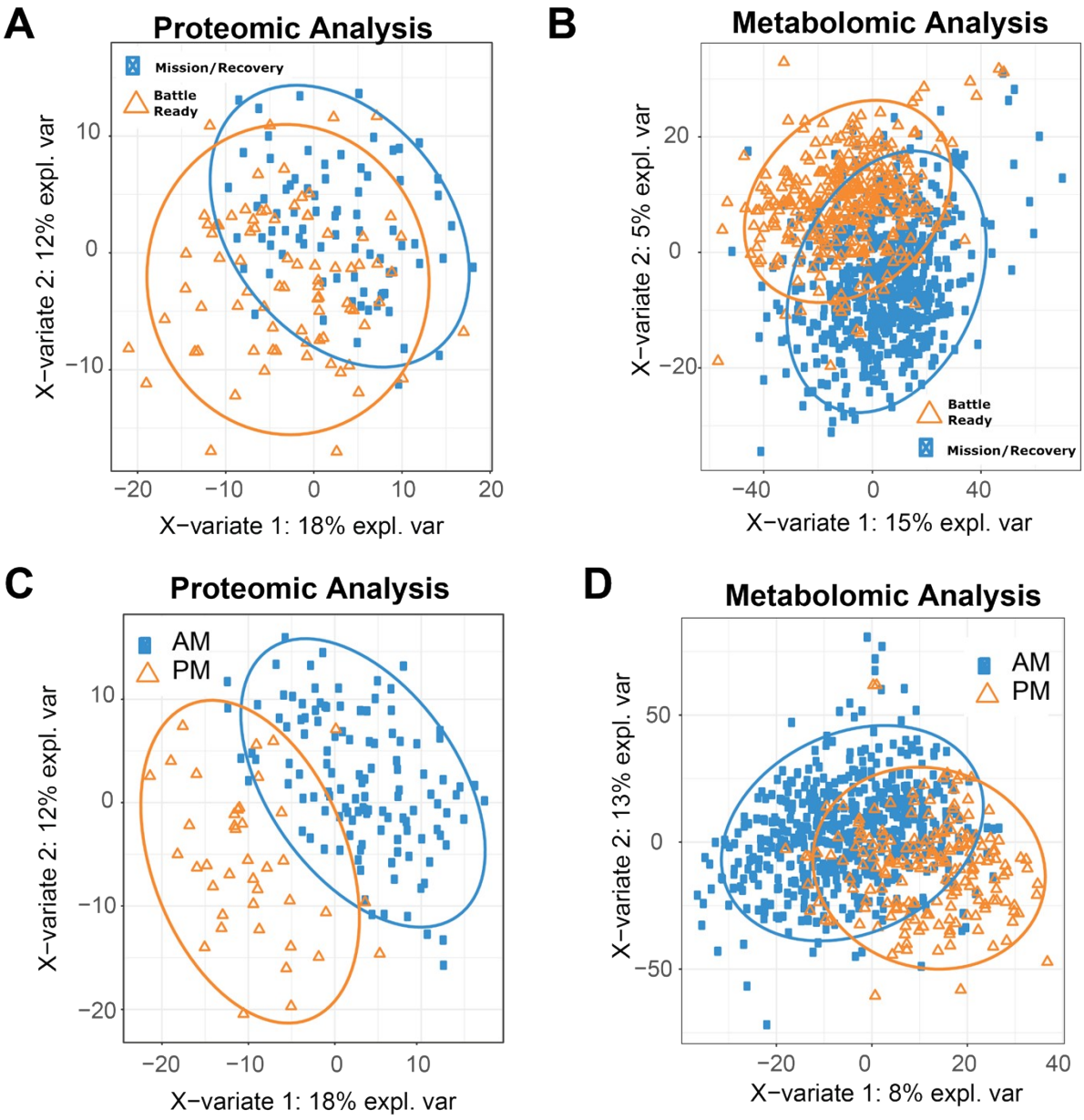
CID#	Compound	HMDB ID
1	Pipecolic Acid	HMDB0000070
2	3-Acetamidobutanal	HMDB0059649
3	1-Piperidine carboxylic acid	HMDB0094697
4	N4-Acetylaminobutanal	HMDB0004226
5	L-trans-4-Methyl-2-pyrrolidinecarboxylic acid	HMDB0029435
6	(2E)-Decenoyl-ACP	HMDB0062225
7	2-Pyrrolidineacetic acid	HMDB0029444
8	N-Methyl-L-proline	HMDB0094696



Supplemental Figure 1: Protein and Peptide Identifications. Number of proteins and peptides identified in each sample with dotted line indicating the mean across all 160 samples. Shaded region shows standard deviation for protein identifications. Protein and peptide identifications do not appear systematically linked to mission or time of day.

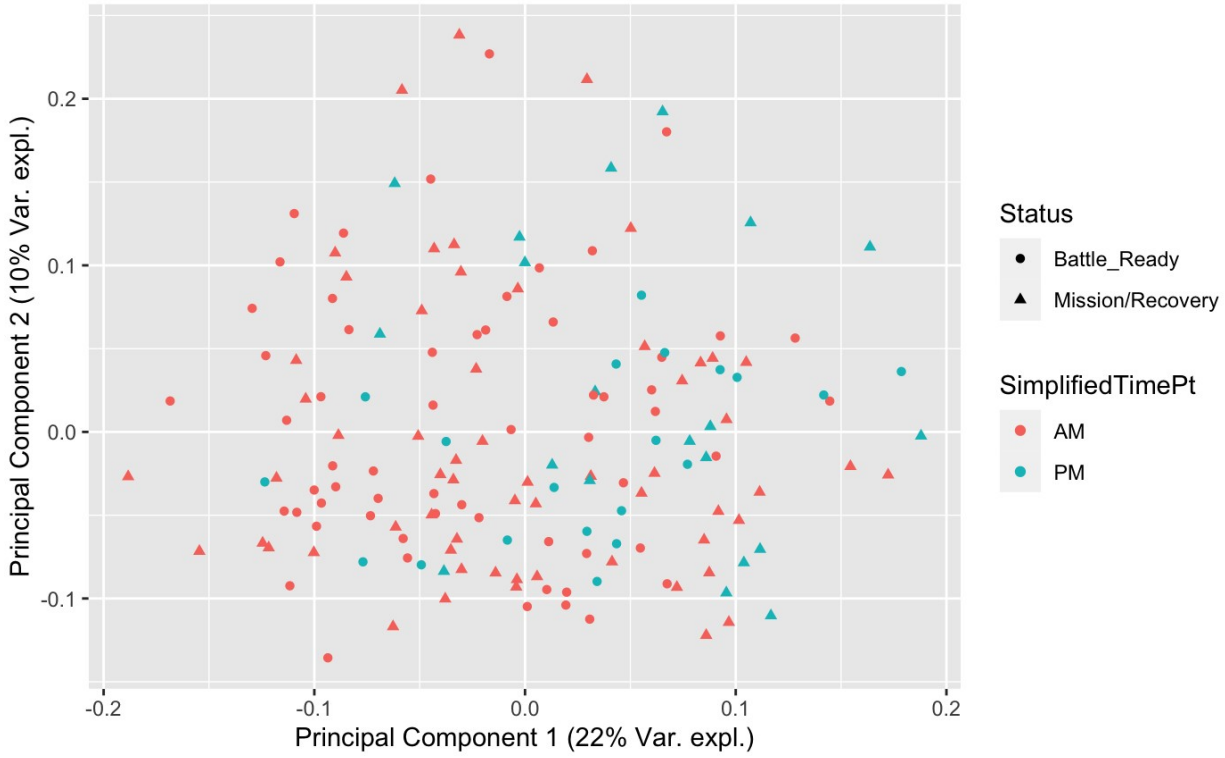


Supplemental Figure 2: Gene Ontology Enrichment. Count and significance of ten most significant biological processes for all proteins identified in any sample. Significance is calculated using a Fisher exact test with full human proteome as background.

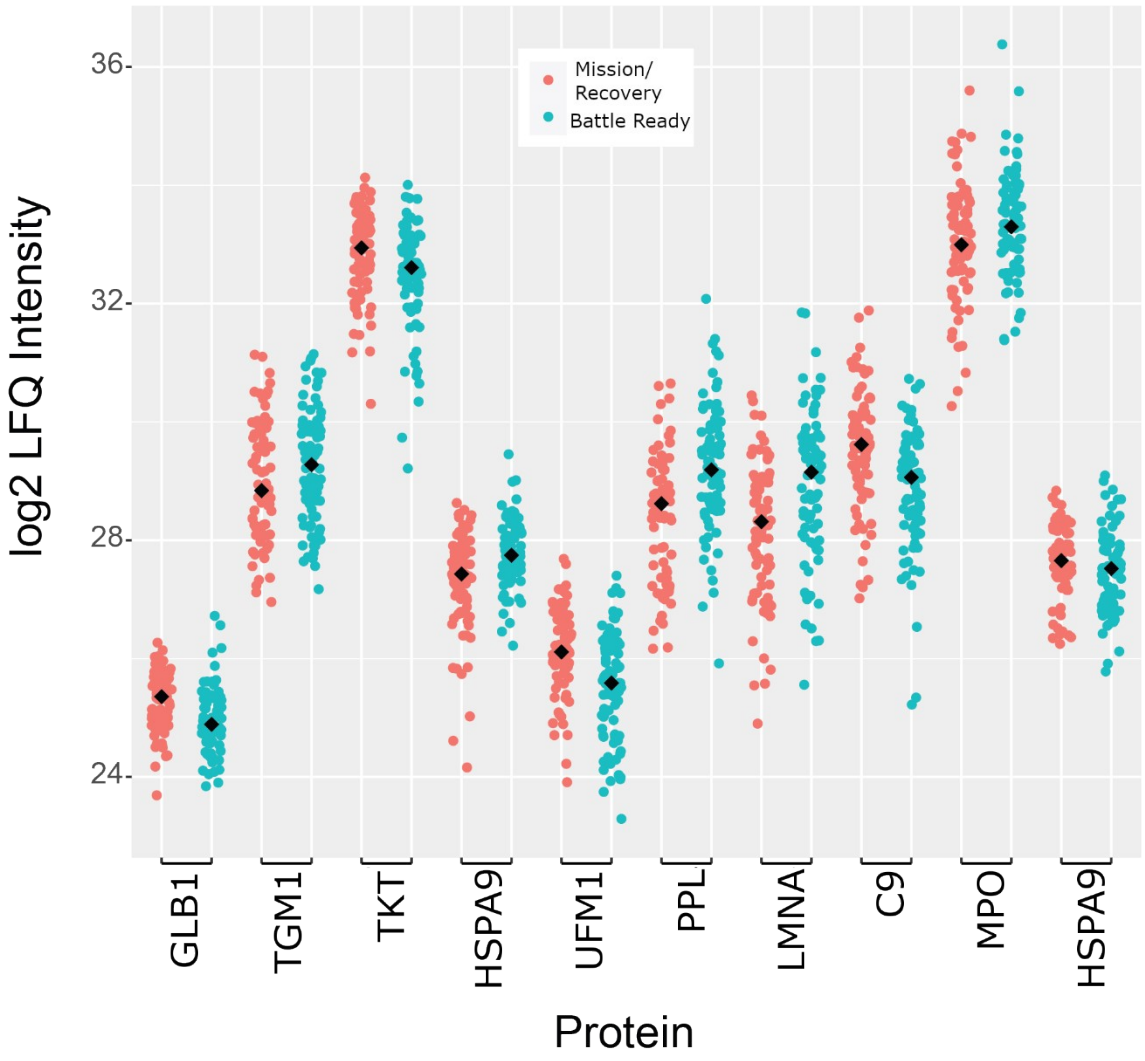


Supplemental Figure 3: Partial Least Squares Discriminant Analysis. (A) Supervised clustering of proteomic samples across initiation of mission (Battle Ready vs Mission/Recovery) based on decomposed values without filtering. (B) Supervised clustering of metabolomic samples across initiation of mission (Battle Ready vs Mission/Recovery) based on decomposed values without filtering. (C) Supervised clustering of proteomic samples by time of day (AM vs PM) based on decomposed values without filtering. PLS-DA separates along time-of-day axis more

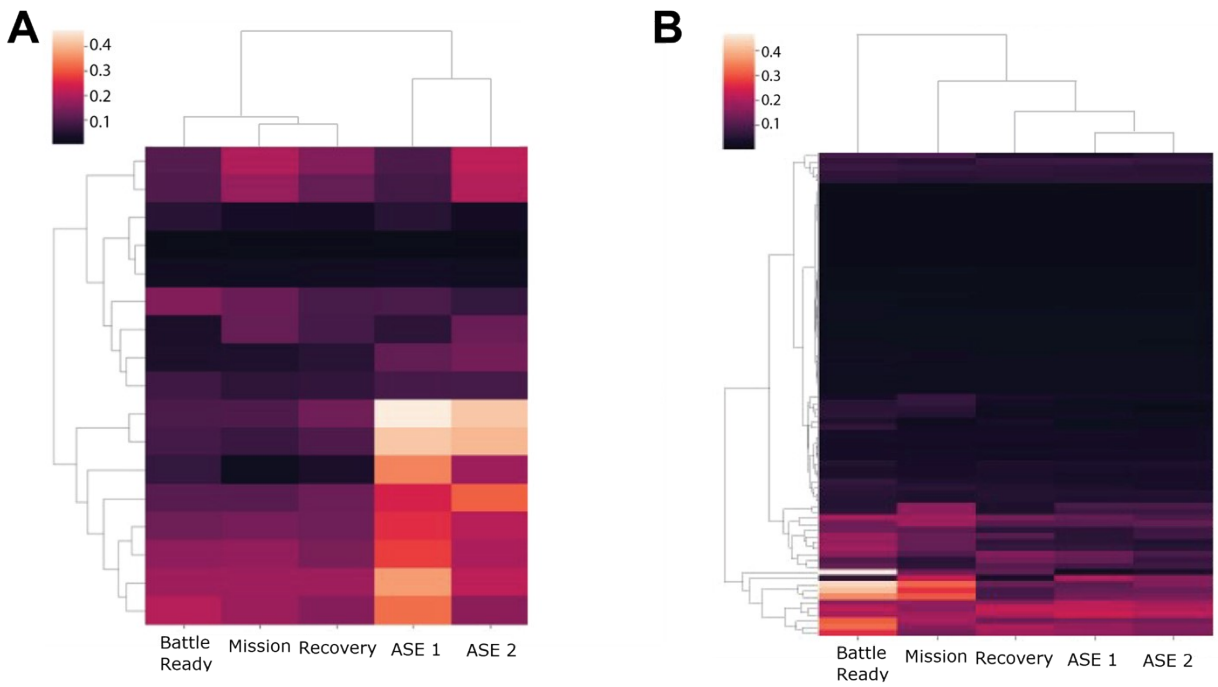
effectively than along mission initiation axis. (D) Supervised clustering of proteomic samples by time of day (AM vs PM) based on decomposed values without filtering. PLS-DA separates along time-of-day axis more effectively than along mission initiation axis.



Supplemental Figure 4: Principal Component Analysis. Unsupervised clustering of proteomic samples by both time of day (AM vs PM) and status (Battle_Ready vs Mission/Recovery).



Supplemental Figure 5: Abundance Shifts for Discriminant Proteins. Log2 transformed LFQ intensities of all samples for five proteins most discriminant for mission initiation [periplakin (PPL), galactosidase beta 1(GLB1) complement component C9 (C9), ubiquitin fold modifier 1 (UFM1) and prelamin A/C (LMNA)] along with proteins from the most discriminant five-protein model[heat shock protein alpha family class B member 1 (HSPAB1), myeloperoxidase (MPO), heat shock protein family A member 9 (HSPA9), and transketolase (TKT)]. Battle Ready samples are colored in blue, while Mission/Recovery samples are colored in red. Black diamonds indicate median intensities for each group.



Supplemental Figure 6: Hierarchical Clustering of Discriminant Metabolites across Time Points.

(A) Heatmap showing hierarchical clustering of compound features associated with arginine biosynthesis. (B) Heatmap showing hierarchical clustering of compounds features associated with histidine metabolism.