1   Milk Metabolomics Data Reveal the Energy Balance of Individual Dairy Cows in Early

2   Lactation

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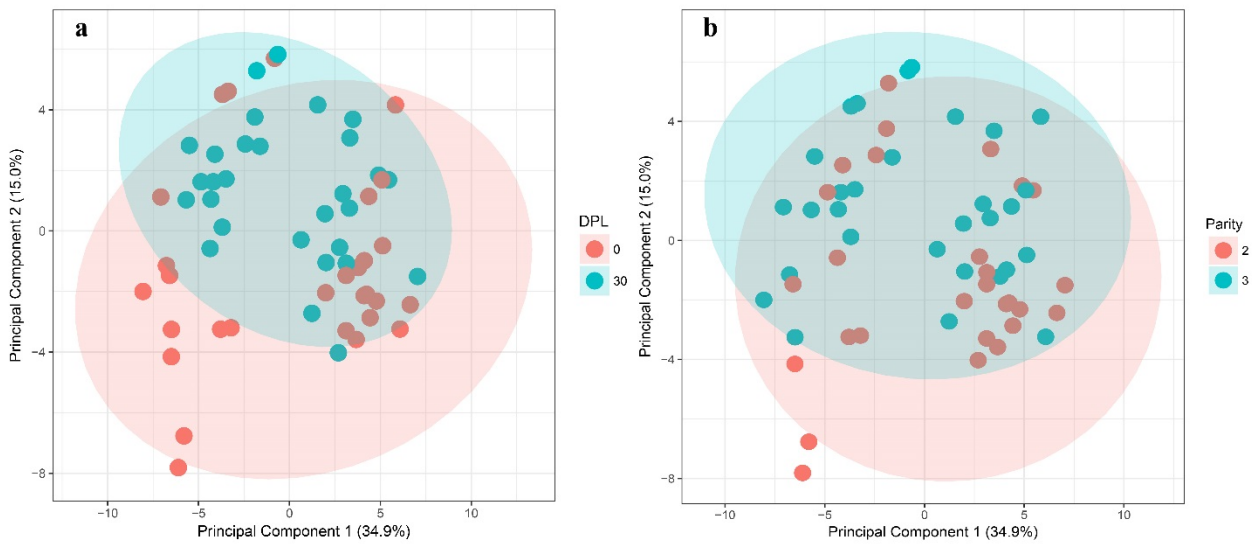5   *of Systems and Synthetic Biology, Wageningen University & Research, Wageningen, the Netherlands*

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Principal Component Analyse

11   Supplementary Fig. S1. Principal component analyses to identify metabotypes, data were labelled with different

12   dry period length (a) and parity (b).

13   Supplementary Fig. S2. Pearson correlations matrix among milk metabolites, milk production traits and energy

14   balance of dairy cows in week 2 (a) and week 7 (b). Blank represents the *P*-value of correlation between two

15   variables is insignificant (*P*-value > 0.05).

16   Abbreviation: cAMP, adenosine 3,5-cyclic monophosphate; AMP, adenosine monophosphate; CMP, cytidine monophosphate; FMN, Flavin

17   mononucleotide; FPCM, fat- and protein-corrected milk production.
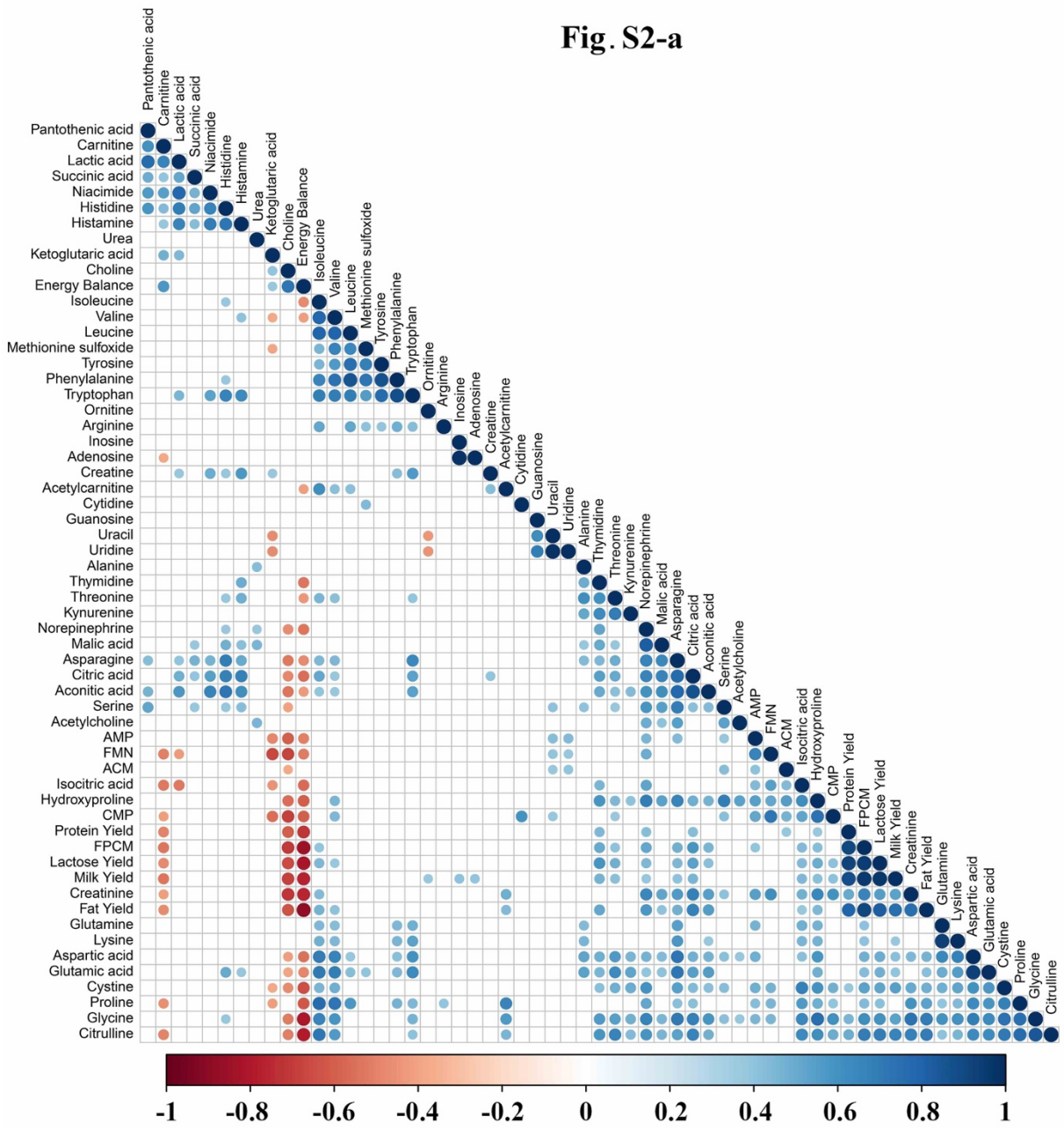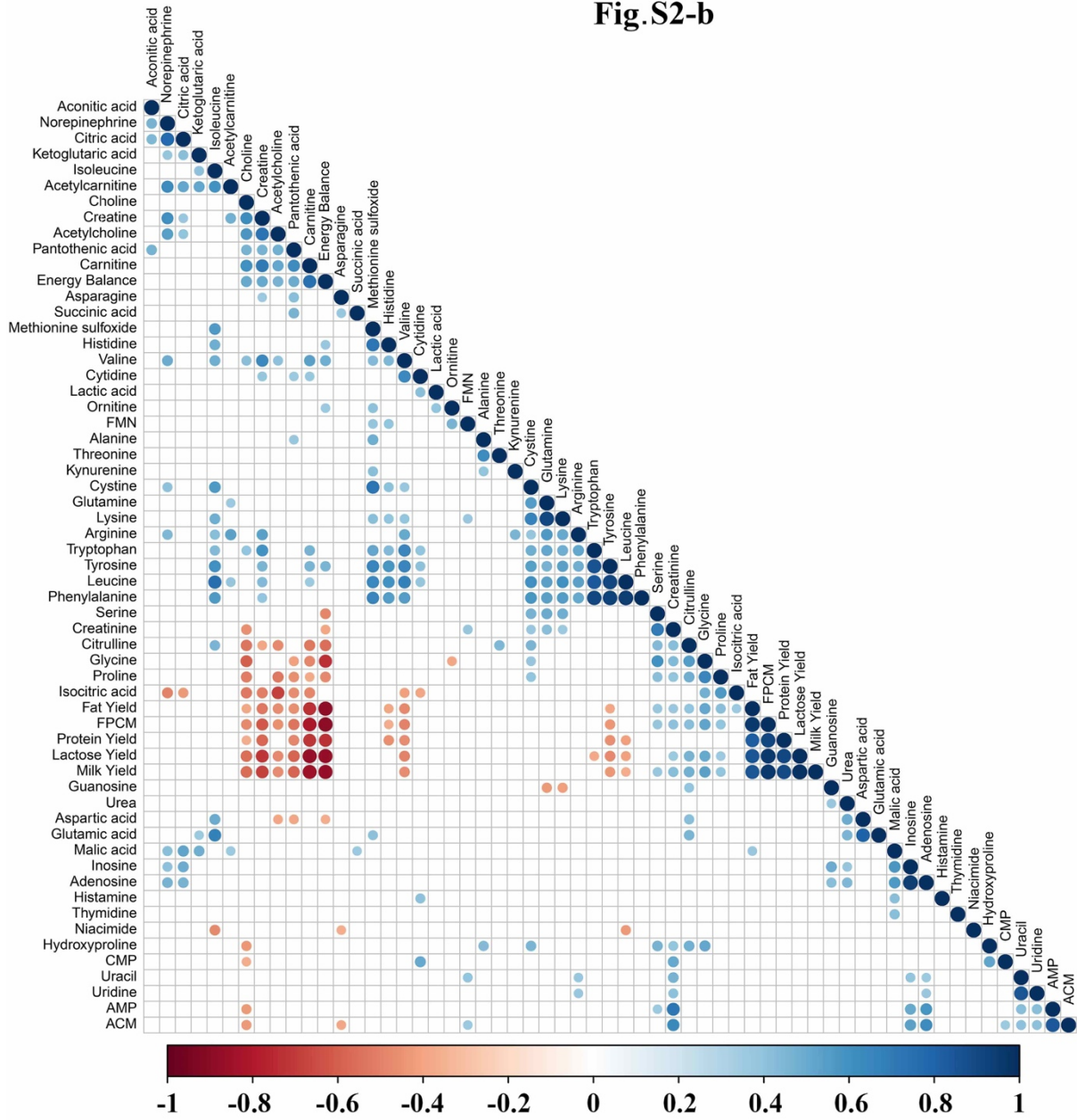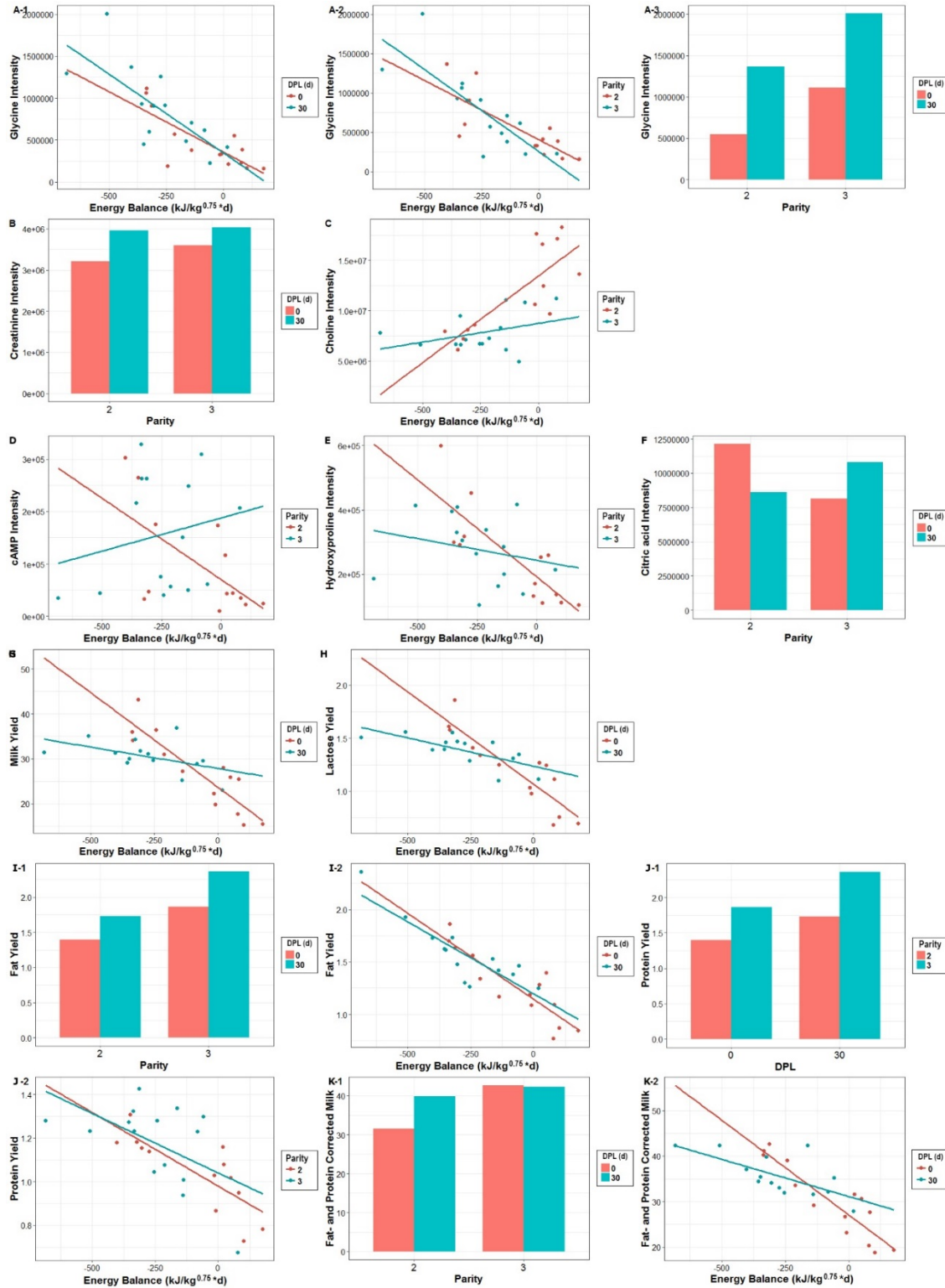
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Fig. S2-a

Fig.S2-b

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23   Supplementary Fig. S3. The effect of significant two-way interaction between energy balance (EB) and different

24   treatments, including dry period (DPL) and parity on in week 2 glycine (A-1, A-2, A-3), Creatinine (B), Choline

25   (C), adenosine 3,5-cyclic monophosphate (cAMP) (D), Hydroxyproline (E), citric acid (F), milk yield (G), lactose

26   (H), fat yield (I-1, I-2), protein (J-1, J-2), FPCM (K-1, K-2).

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Supplementary Fig. S4. The effect of significant two-way interaction between EB and different treatments, including dry period (DP) and parity in week 7 on glycine (A-1, A-2), Citrulline (B-1, B-2), Tyrosine (C-1, C-2, C-3), lactose (D), protein (E), FPCM (F).