

**Supplementary information S1: Comparison of PSG-assessed sleep traits in subjects with insomnia and good sleepers. Means and SD provided.**

<b>PSG variable</b>	<b>Insomnia</b>	<b>Good Sleeper</b>
Sleep latency (minutes)	25.6 (22.8)	22.3 (36.8)
Wakefulness after sleep onset (minutes)	113.7 (84.0)	81.5 (55.7)
Sleep efficiency	75.8% (14.6%)	80.7% (9.8%)
Total sleep time (minutes)	428.5 (98.1)	435.3 (78.2)
% of sleep time spent in Stage N1 sleep	13.6% (5.5%)	15.0% (5.6%)
% of sleep time spent in Stage N2 sleep	47.1% (6.2%)	48.7% (9.9%)
% of sleep time spent in Stage N3 sleep	17.9% (7.5%)	16.7% (5.1%)
% of sleep time spent in Stage REM sleep*	21.5% (4.8%)	19.7% (8.7%)

\* p<0.05

**Supplementary information S2: Loadings and VIP values of metabolites from different multivariate OPLS-DA models.**

<b>All timepoints taken together</b>					
Metabolite	Loadings	VIP	Metabolite	Loadings	VIP
Isoleucine	-0.05	1.62	2-Hydroxyisovalerate	0.04	1.63
Lysine	-0.03	1.29	2-Oxoisocaproate	0.02	1.25
Acetate	-0.03	1.48	2-Oxovalerate	0.01	1.12
Valine	-0.004	1.04	3-Methyl-2-oxovalerate	0.02	1.22
Pyruvate	-0.02	1.18	Propylene glycol	0.04	1.4
3-Hydroxybutyrate	-0.02	1.35	N-acetyl metabolites	0.02	1.27
Citrate	-0.02	1.31	Proline	0.06	2.03
Dimethylamine	-0.005	1.09	Phenylalanine	0.03	1.47
Dimethylglycine	-0.004	1.08	p-Methylhistidine	0.04	1.28
Ornithine	-0.02	1.31			
Serine	-0.02	1.26			
Creatinine	-0.03	1.32			
Tyrosine	-0.02	1.13			
<b>9 am - 5 pm timepoints</b>					
Metabolite	Loadings	VIP	Metabolite	Loadings	VIP
Valine	-0.03	1.3	Propylene glycol	0.04	1.41
Isoleucine	-0.02	1.1	Lactate	0.02	1.38
Lysine	-0.02	1.24	N-Acetyl metabolites	0.02	1.24
Acetate	-0.03	1.4	Glutamate	0.06	2.02

3-Hydroxybutyrate	-0.005	1.05	Glycine	0.004	1.01
Proline	-0.02	1.22	Tryptophan	0.04	1.46
Pyruvate	-0.02	1.12	Phenylalanine	0.02	1.33
Pyroglutamate	-0.03	1.37	p-Methylhistidine	0.05	1.57
Glutamine	-0.01	1.14			
Citrate	-0.01	1.16			
Ornithine	-0.02	1.38			
Creatine	-0.02	1.37			
Creatinine	-0.02	1.23			
Serine	-0.03	1.26			
Tyrosine	-0.03	1.24			

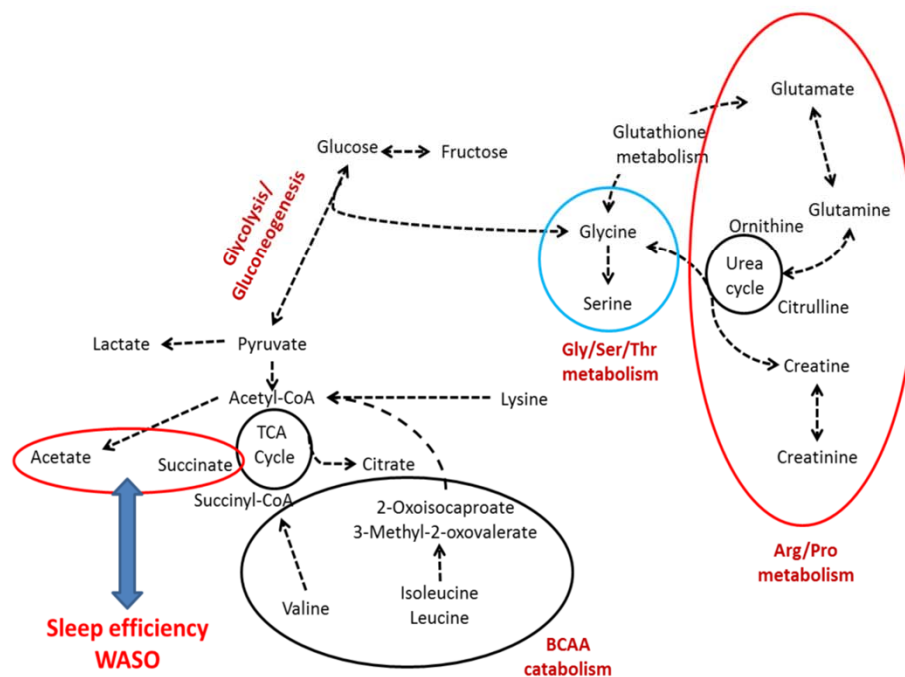
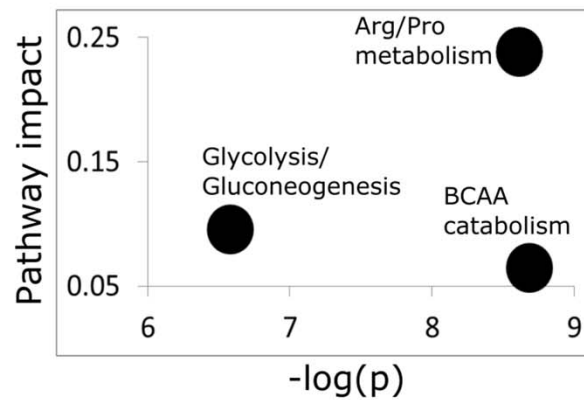
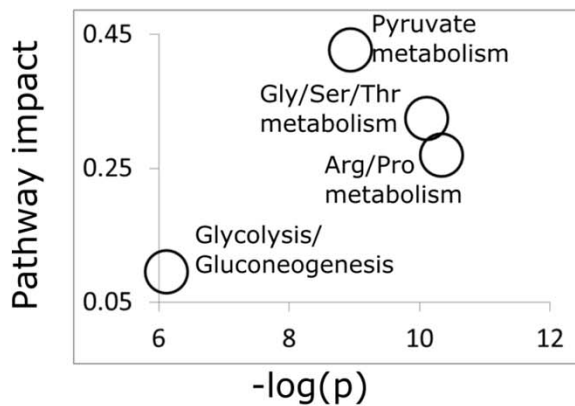
### 11 pm - 7 am timepoints

Metabolite	Loadings	VIP	Metabolite	Loadings	VIP
Lysine	-0.03	1.23	2-Oxoisocaproate	0.04	1.51
Acetate	-0.02	1.23	3-Methyl-2-oxovalerate	0.01	1.06
Valine	-0.006	1.02	Isoleucine	0.02	1.19
Glutamine	-0.03	1.3	Lactate	0.03	1.37
Citrate	-0.01	1.1	Leucine	0.02	1.35
Dimethylamine	-0.009	1.09	N-Acetyl metabolites	0.03	1.26
Creatinine	-0.03	1.23	Proline	0.03	1.28
Ornithine	-0.02	1.19			
Pyruvate	-0.02	1.15			
Glucose	-0.02	1.27			

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Fructose	-0.03	1.35
3-Hydroxybutyrate	-0.03	1.29
Tyrosine	-0.02	1.06

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**Supplementary Table S4: AUC analysis of carbohydrate metabolites and branched chain amino acids in insomnia and control group across nighttime normalized to 11 pm concentration. Figure 4 shows the temporal change of the metabolites. Only second night is considered for the analysis.**

<b>AUC</b>	<b>Control</b>	<b>Insomnia</b>	<b>Fold change</b>
<b>Carbohydrate metabolites</b>			
<b>Glucose</b>	29971.30	32649.34	1.09
<b>Acetate</b>	581.20	659.50	1.13
<b>Tyrosine</b>	450.00	519.24	1.15
<b>Branched chain amino acid metabolite</b>			
<b>2-Oxoisocaproate</b>	287.12	262.77	0.91

