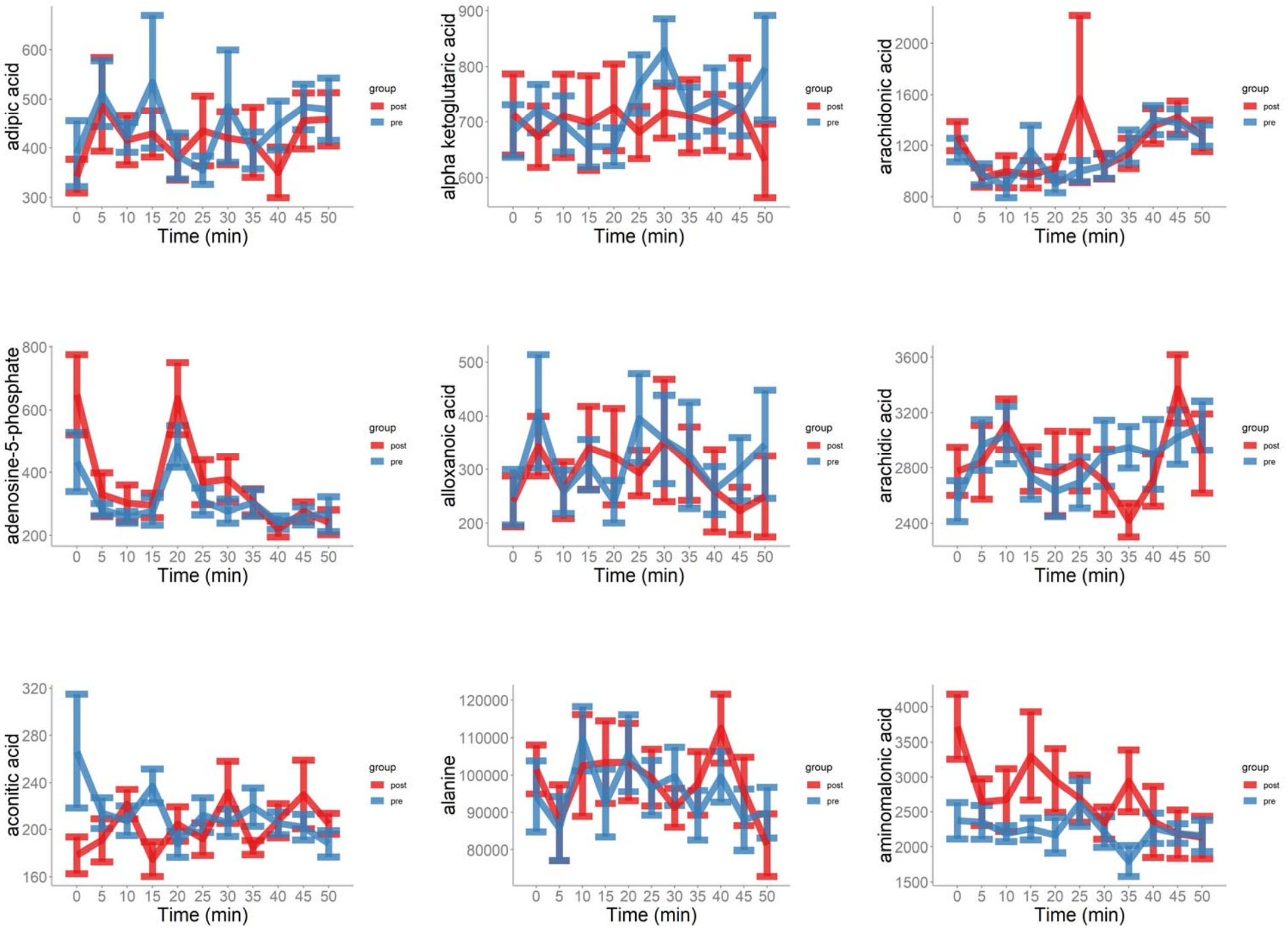
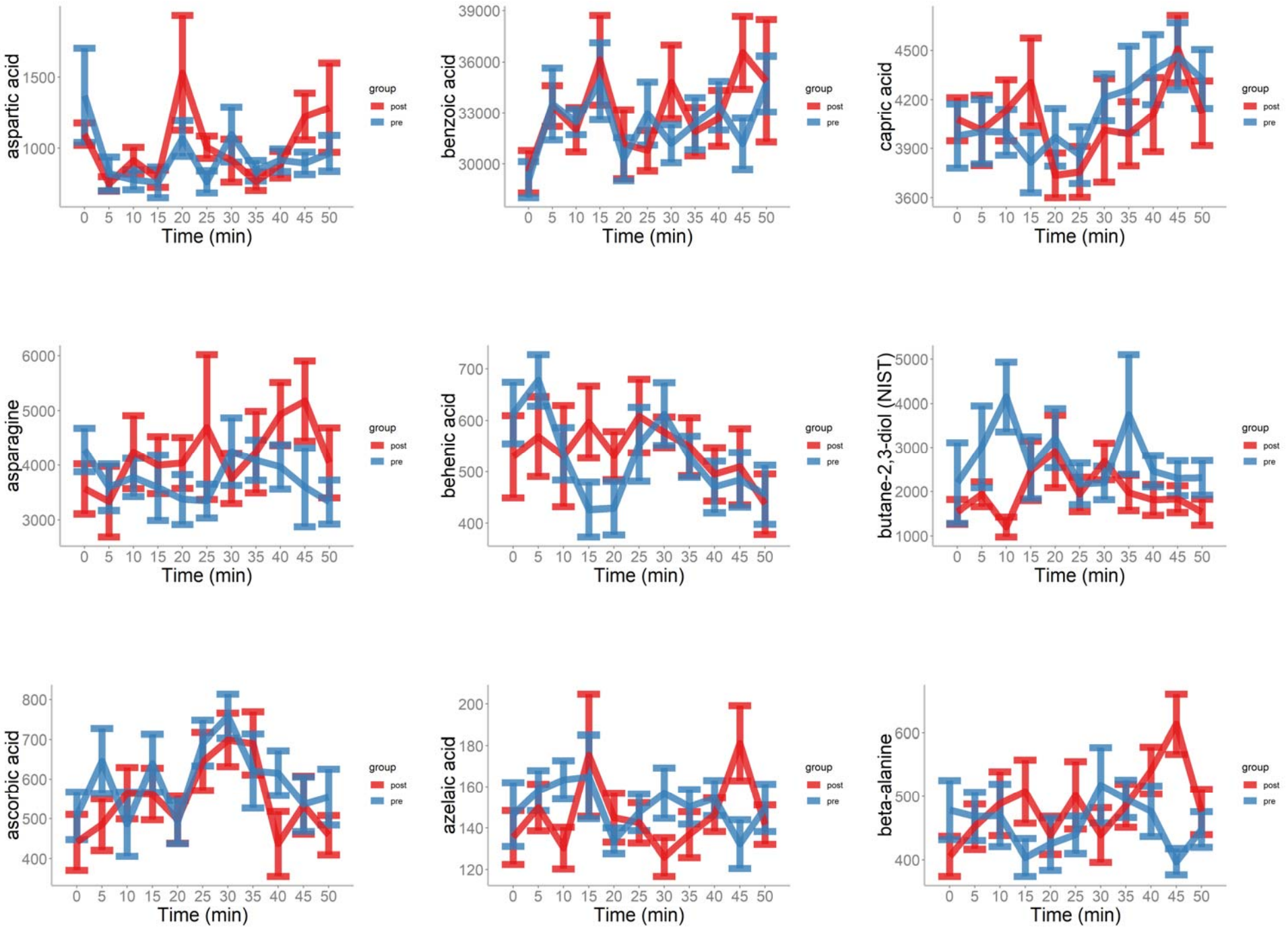
Supporting Materials 1A (Grapov et al.)– Individual annotated metabolite concentration excursions during 30 min. fixed-workload exercise (ergonomic cycle) and 20 min. recovery in adult obese, sedentary, insulin-resistant women, before (pre-, n=15) and after (post-, n=12) a ~14 week weight loss and fitness regimen that significantly improved metabolic health. Concentrations are derived from metabolomics analysis and depicted here as means ± SEM based on quantifier peak ion heights.

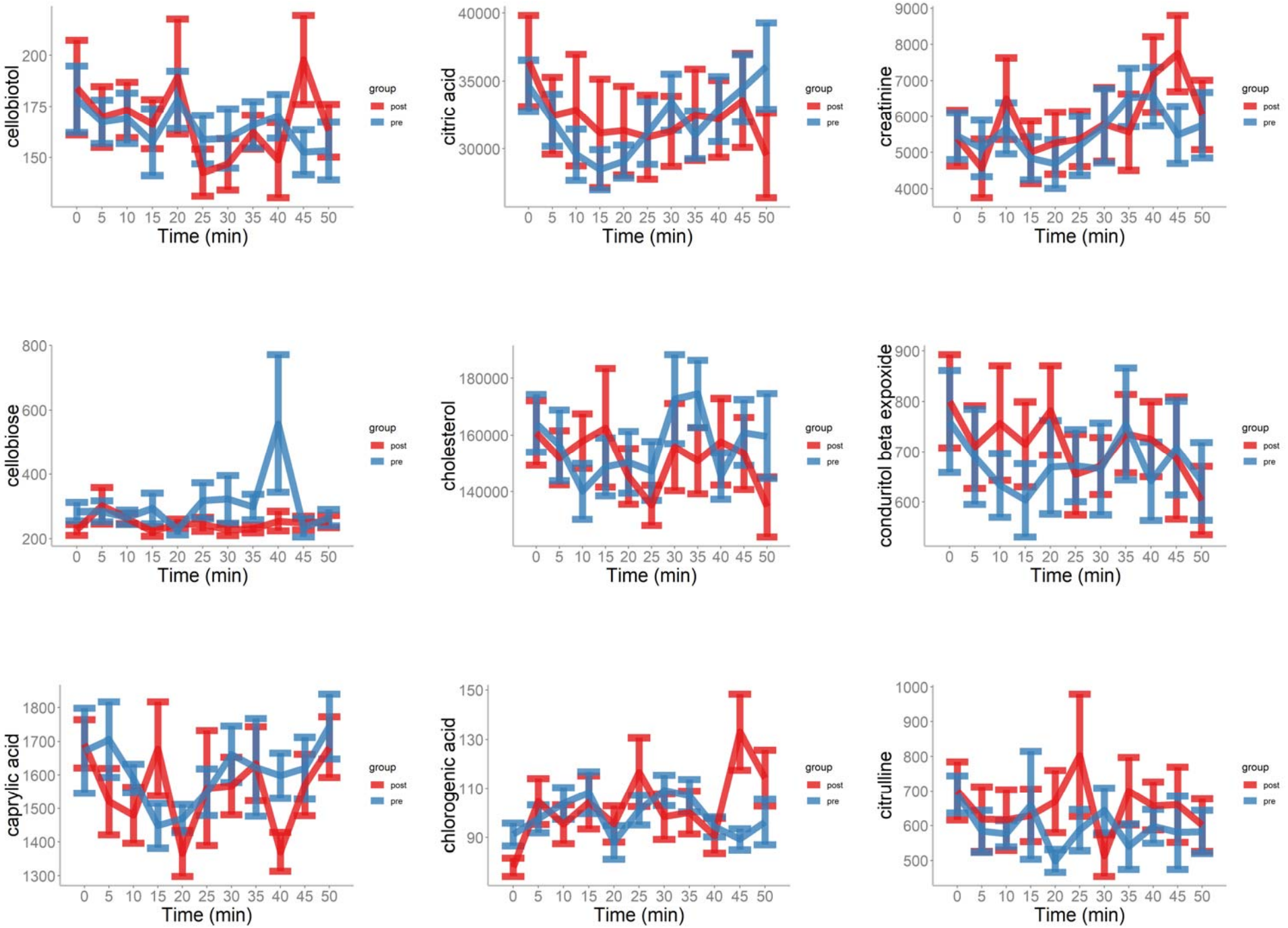
Supporting Materials 1B (Grapov et al.)– NOTE: THIS SET OF FIGURES WITH A SINGLE SOLID LINE TRACKING EXCURSIONS OF INDIVIDUAL METABOLITES FOLLOWS THE 1A FIGURES THAT HAVE 2 LINES (BLUE AND RED). Individual annotated metabolite concentration excursions during 30 min. fixed-workload exercise (ergonomic cycle) and 20 min. recovery in adult obese, sedentary, insulin-resistant women, using data combined from before and after a ~14 week weight loss and fitness regimen. Residuals were used from linear model for intervention (intervention-adjusted) over the measured time points (see Methods in the main paper). Concentrations are semi-quantitative and derived from metabolomics analysis and depicted here as means ± SEM based on quantifier peak ion heights.



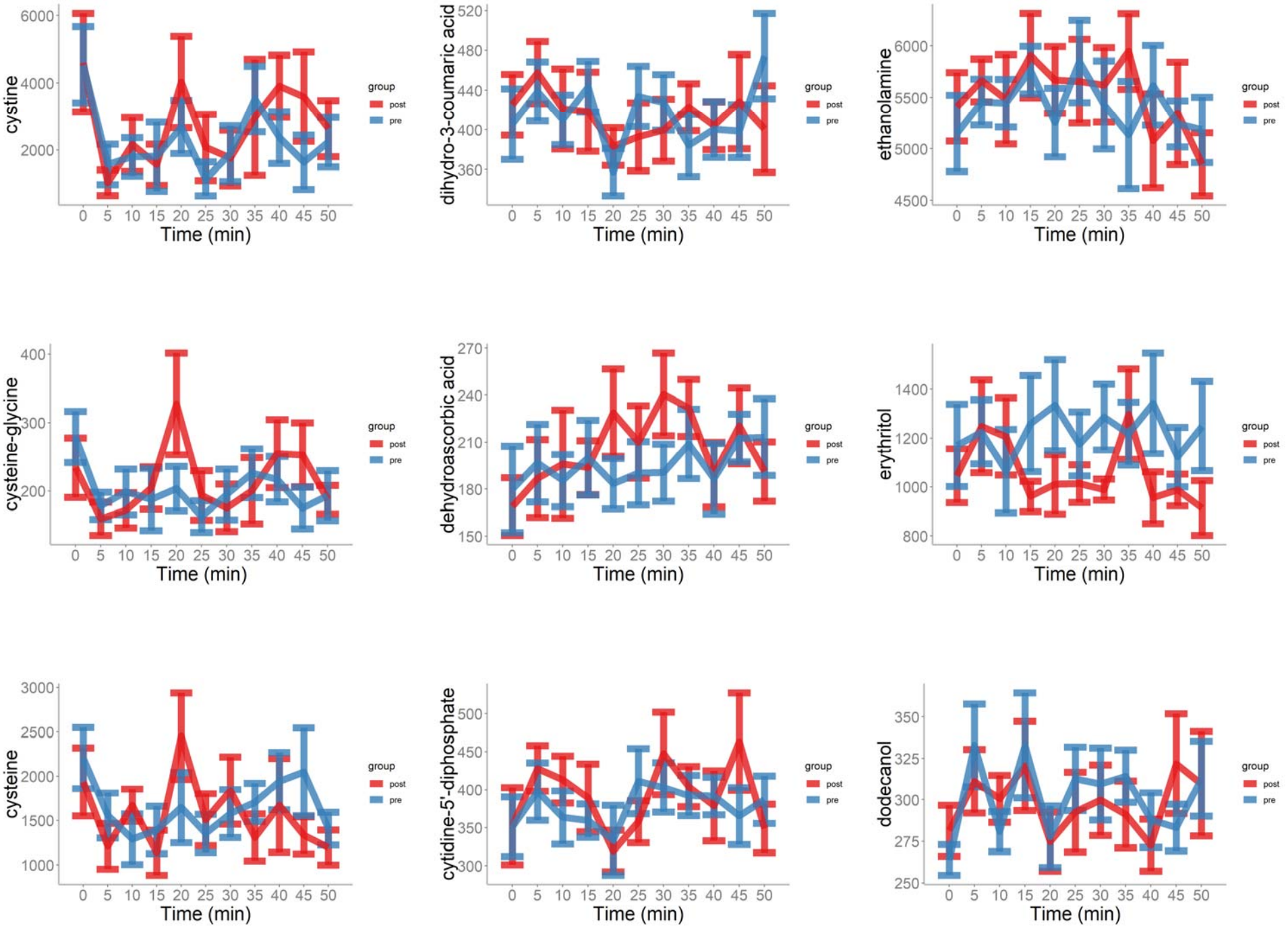
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



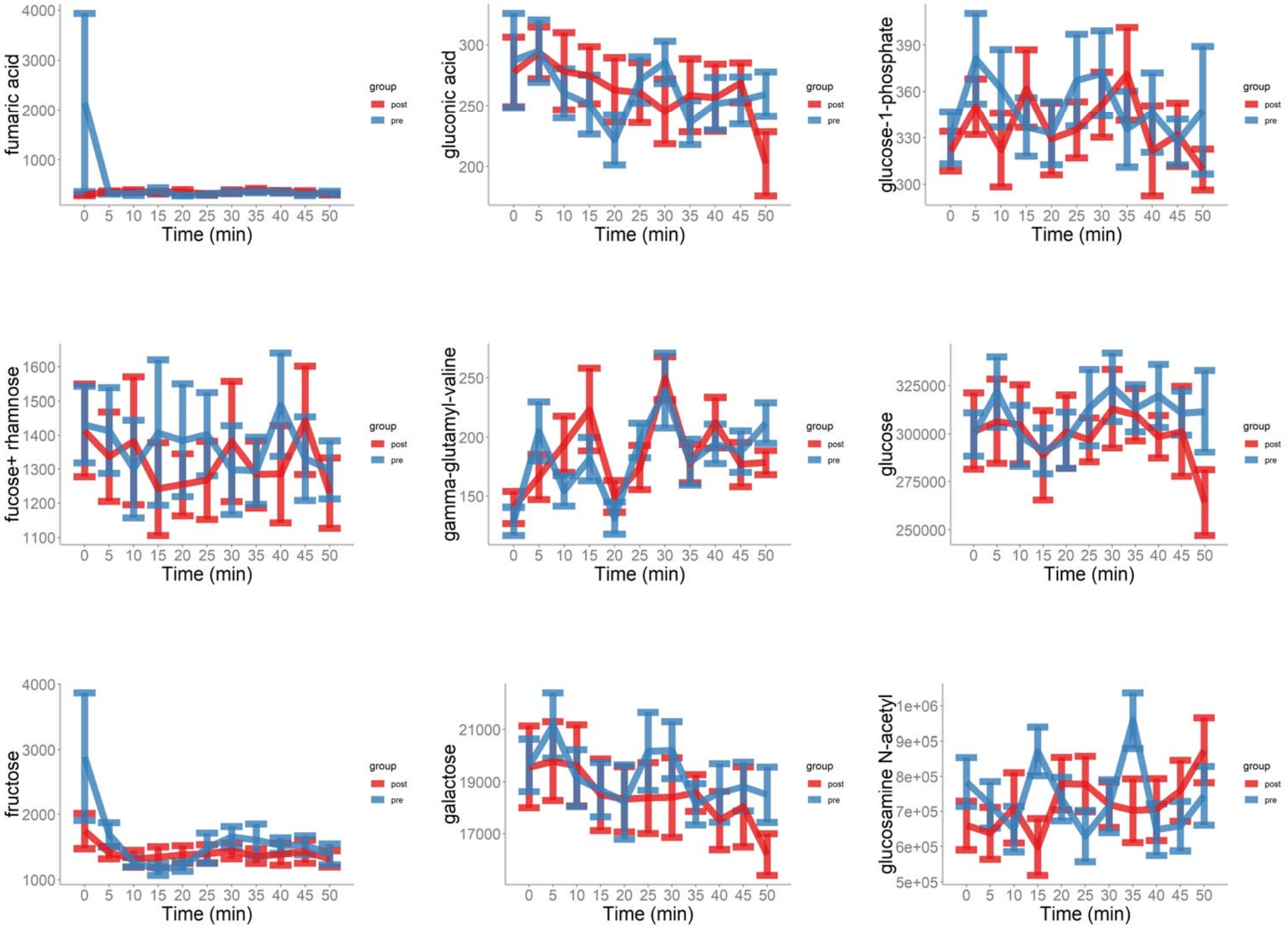
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



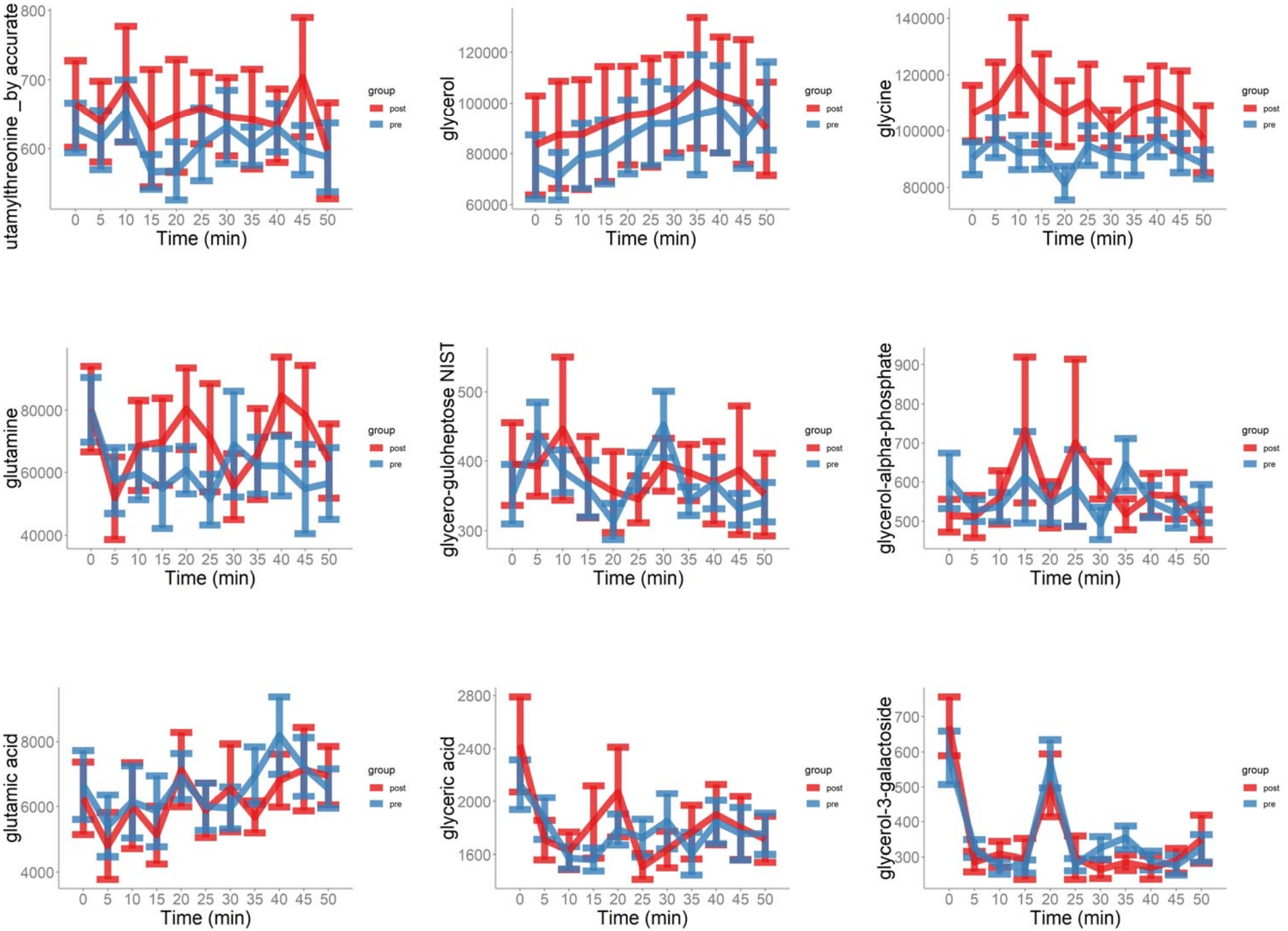
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



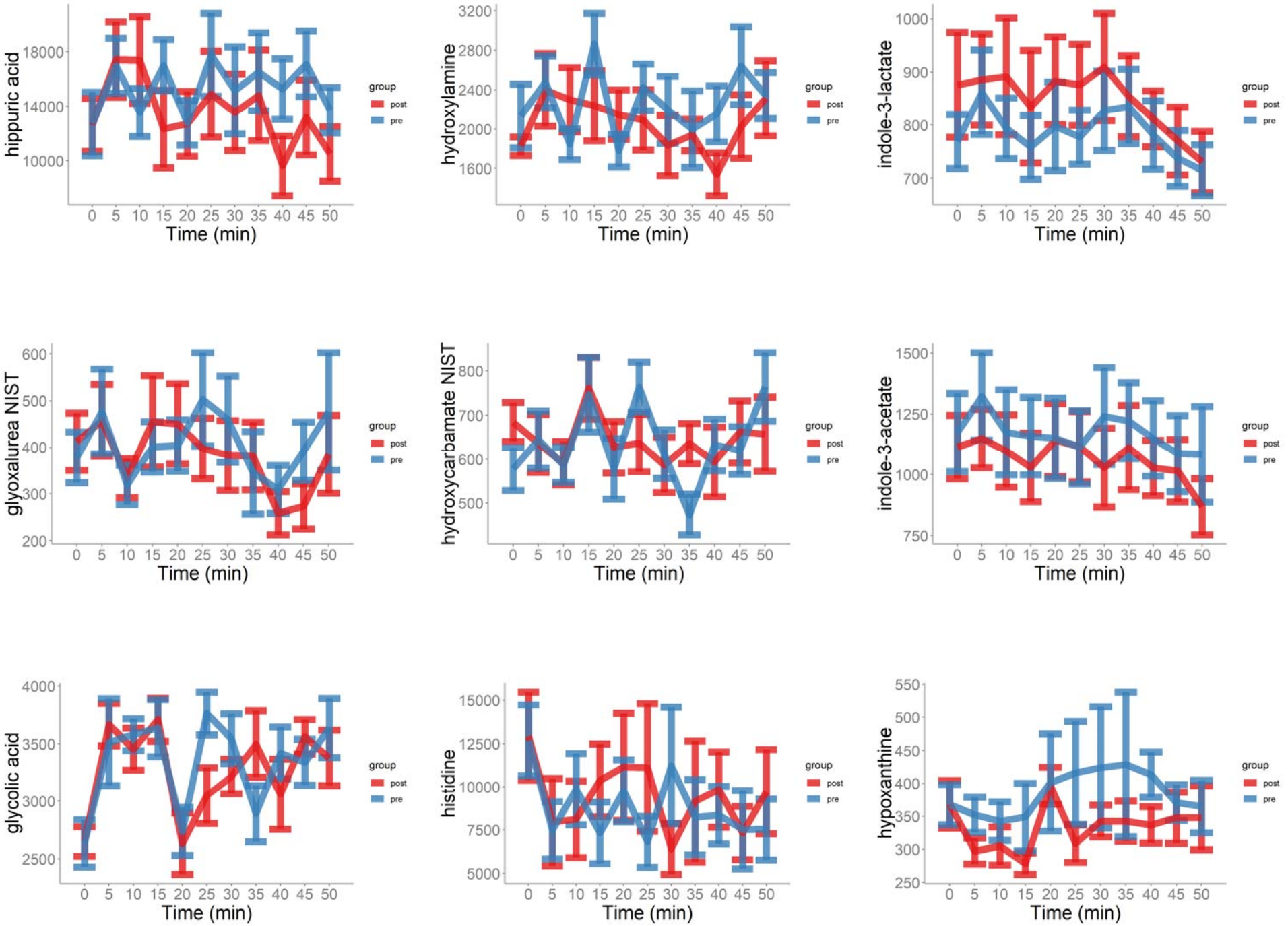
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



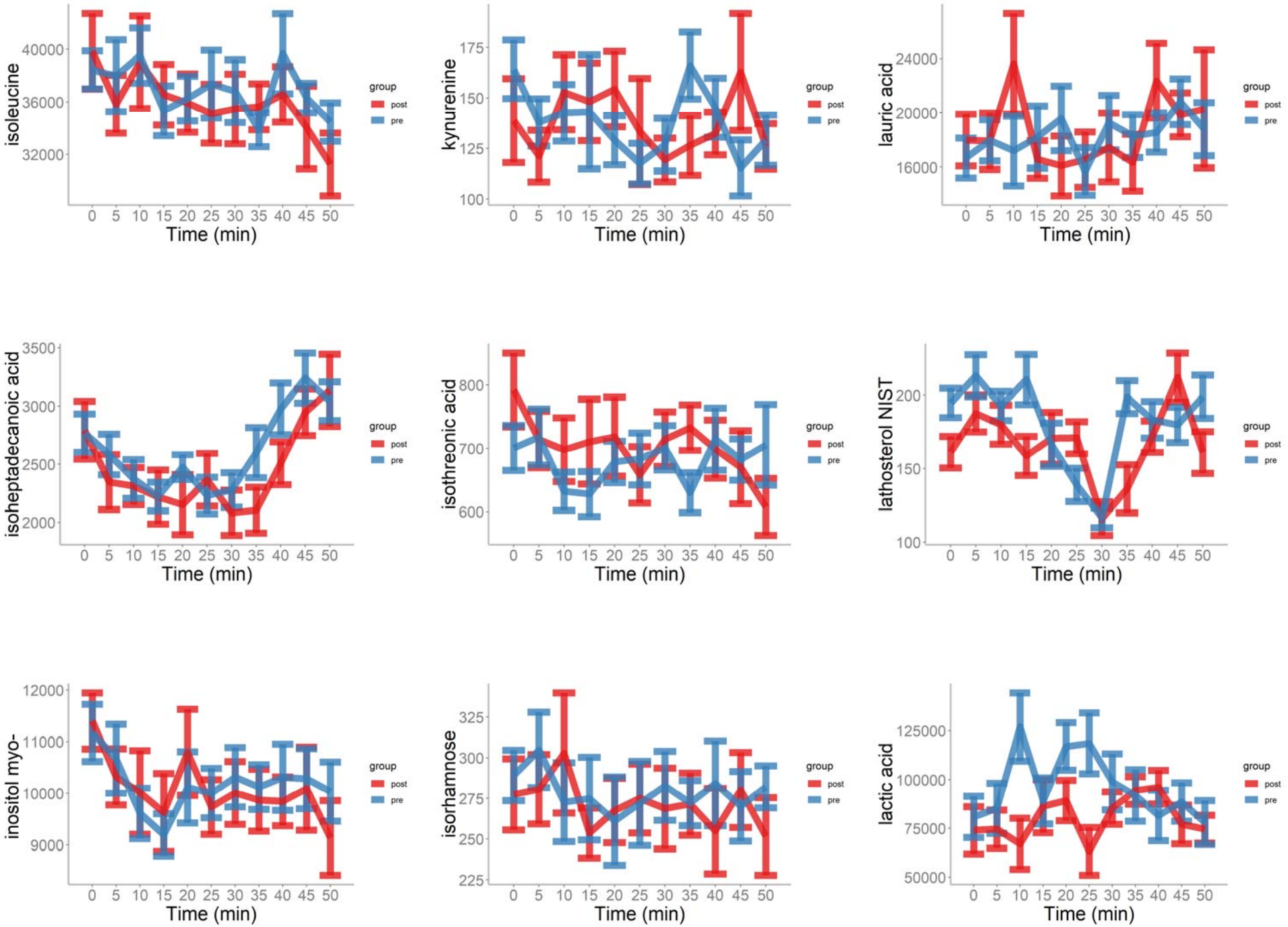
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



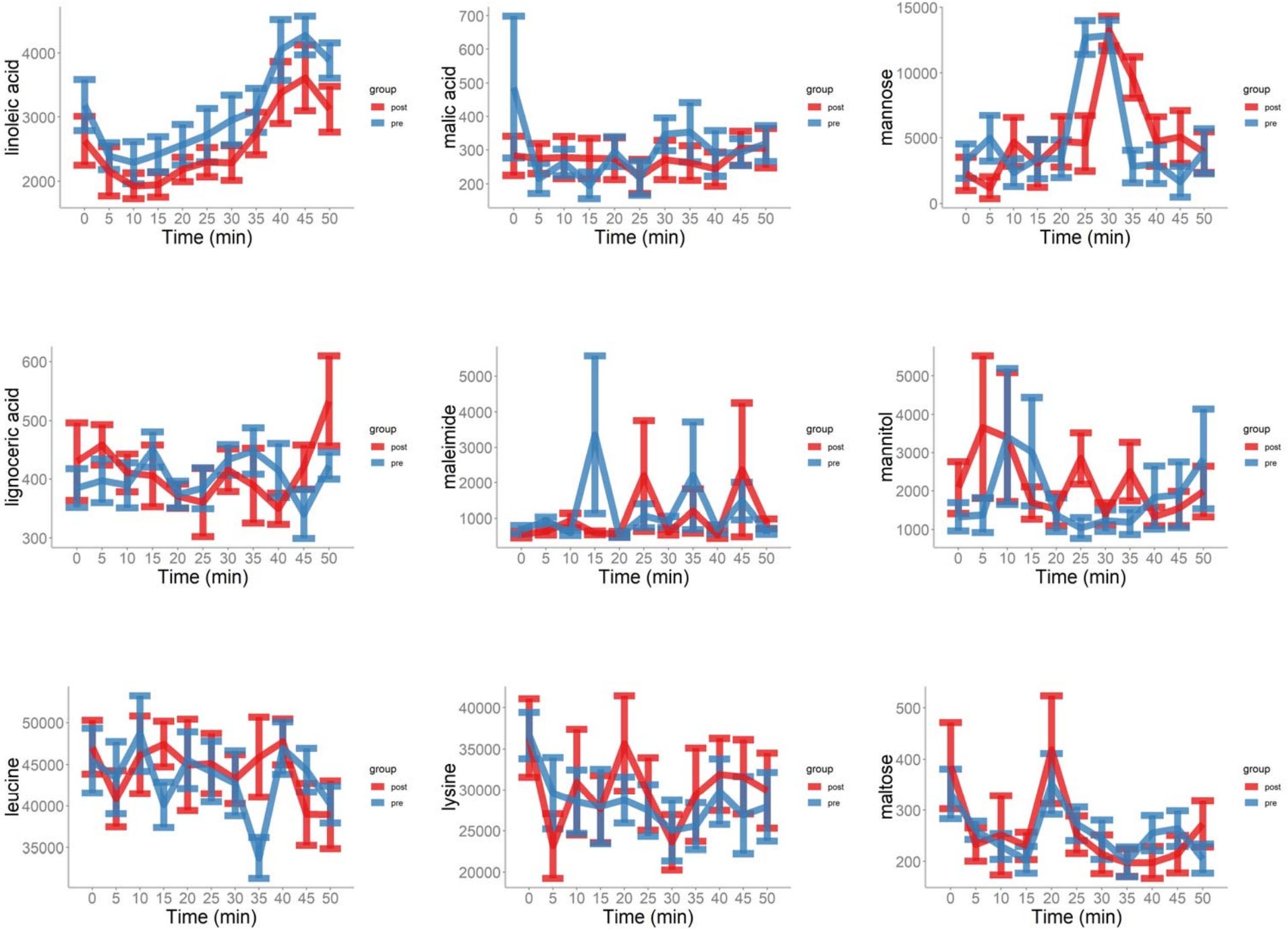
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



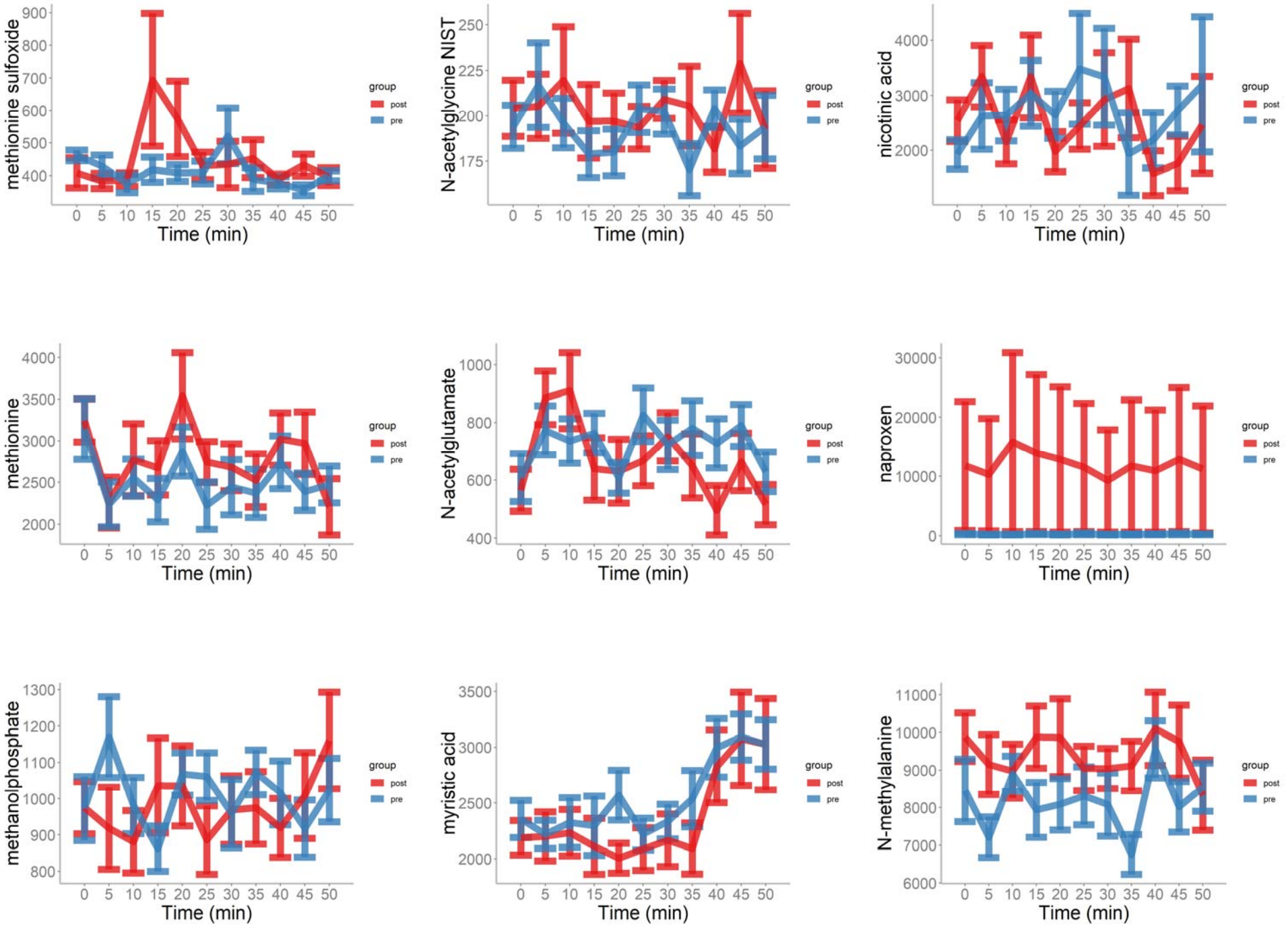
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



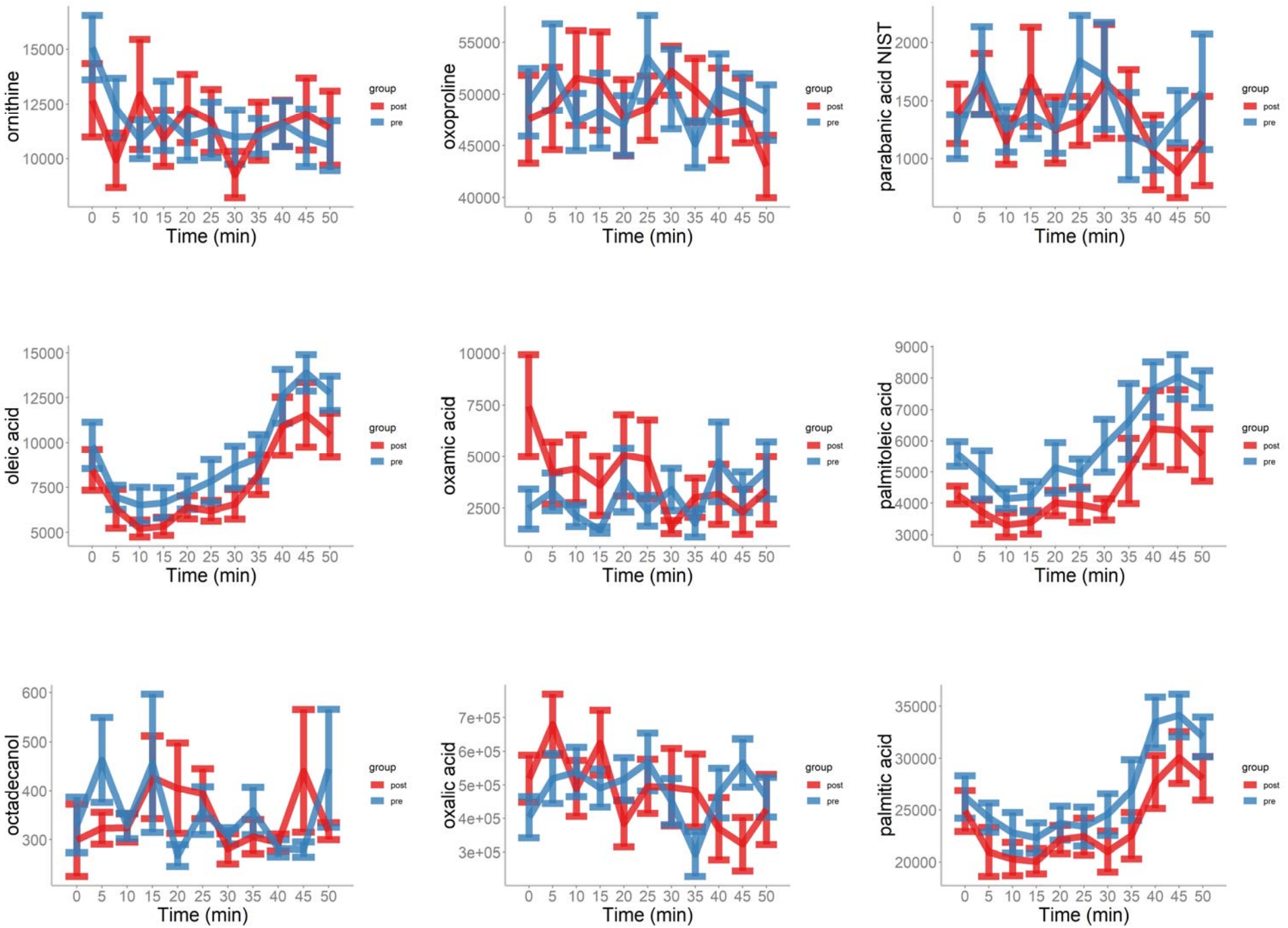
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



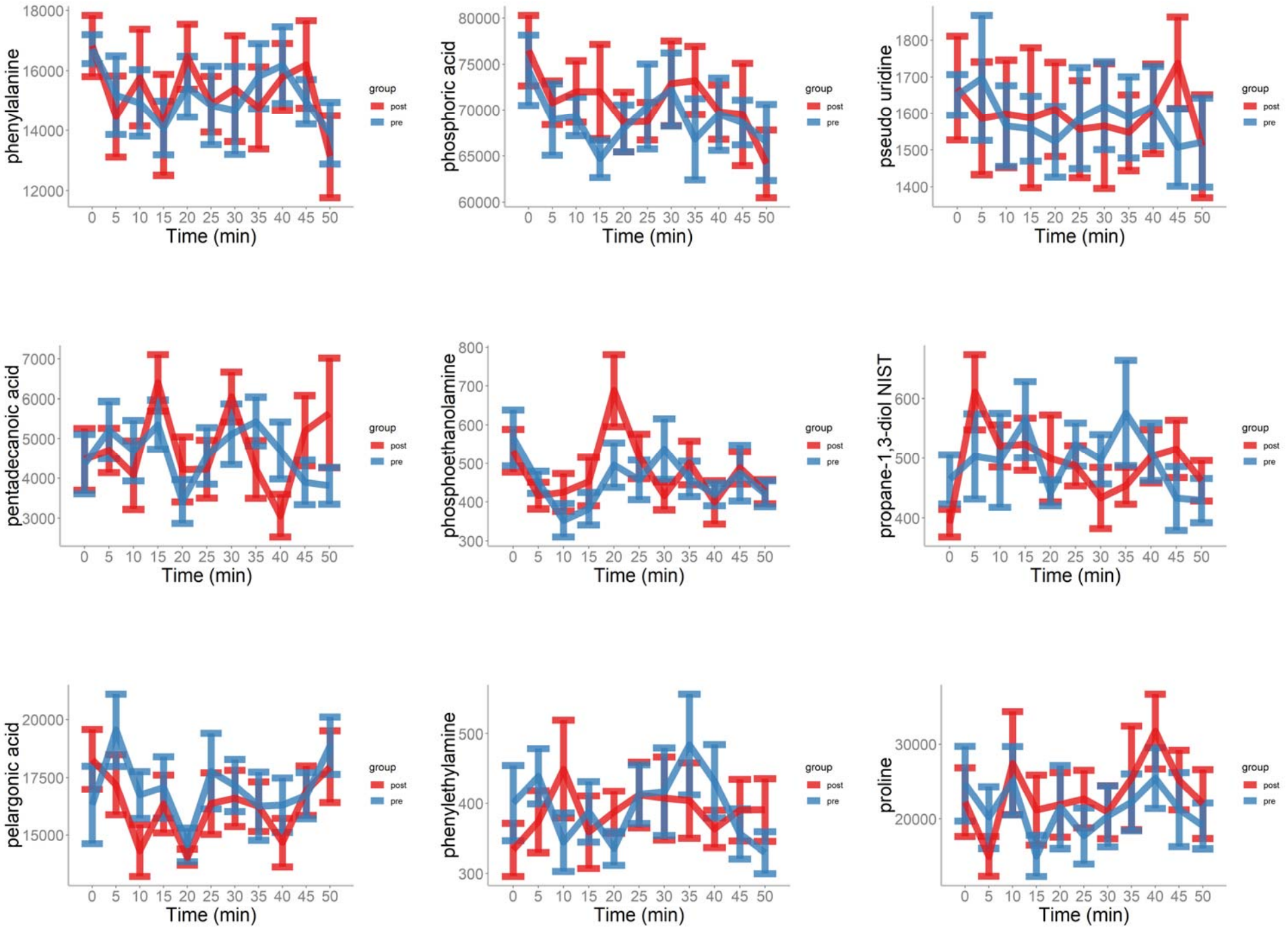
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



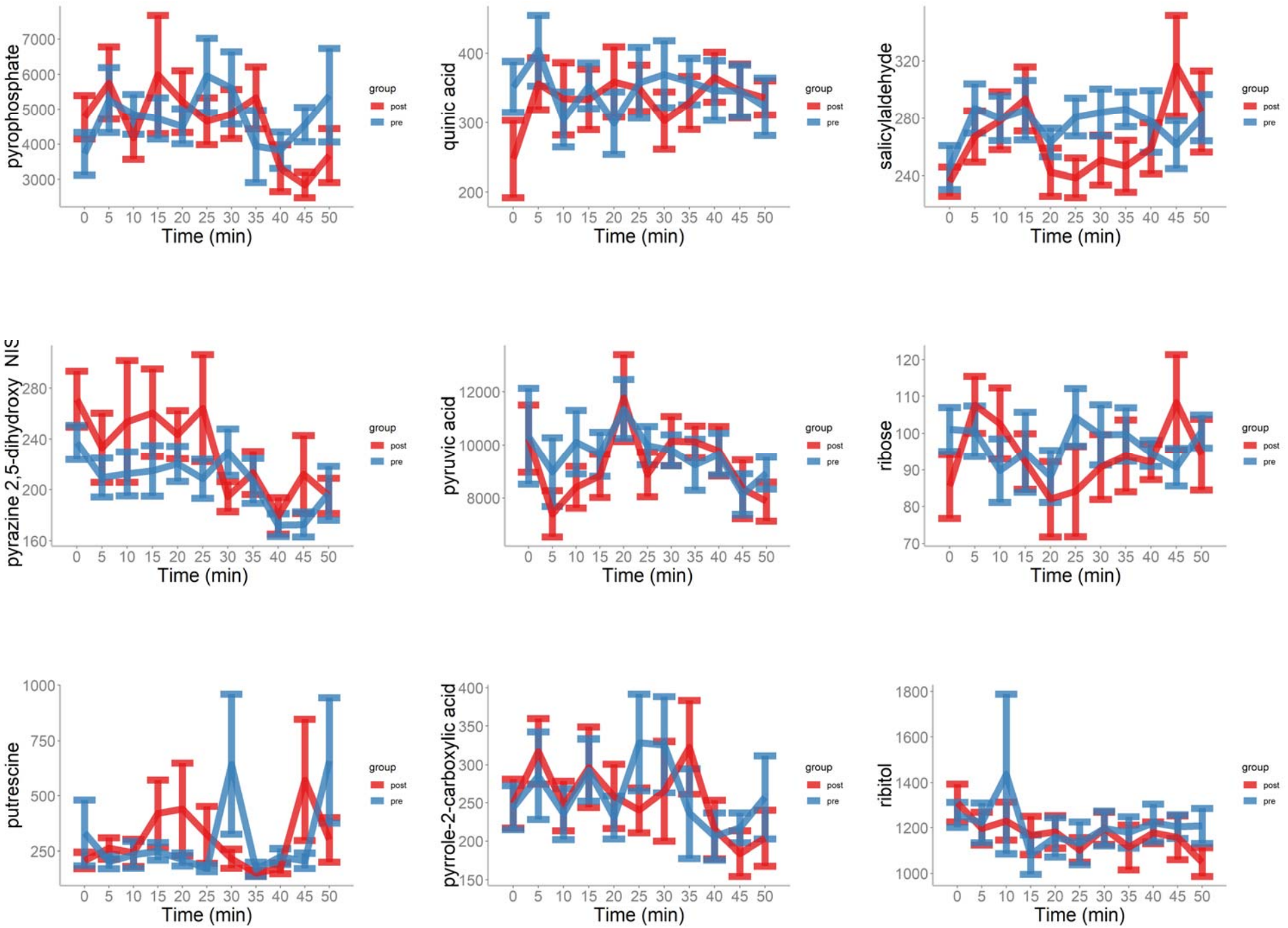
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



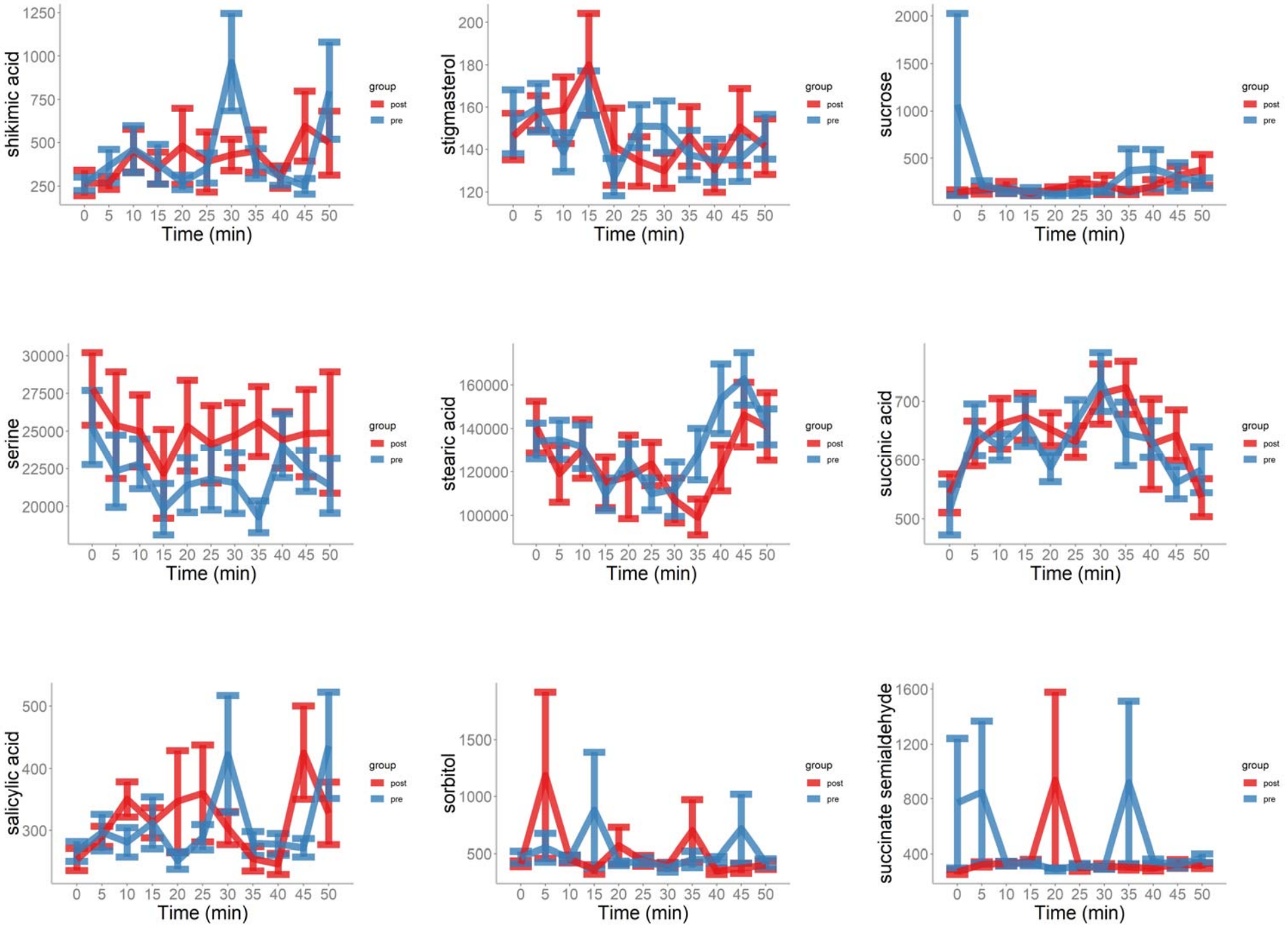
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



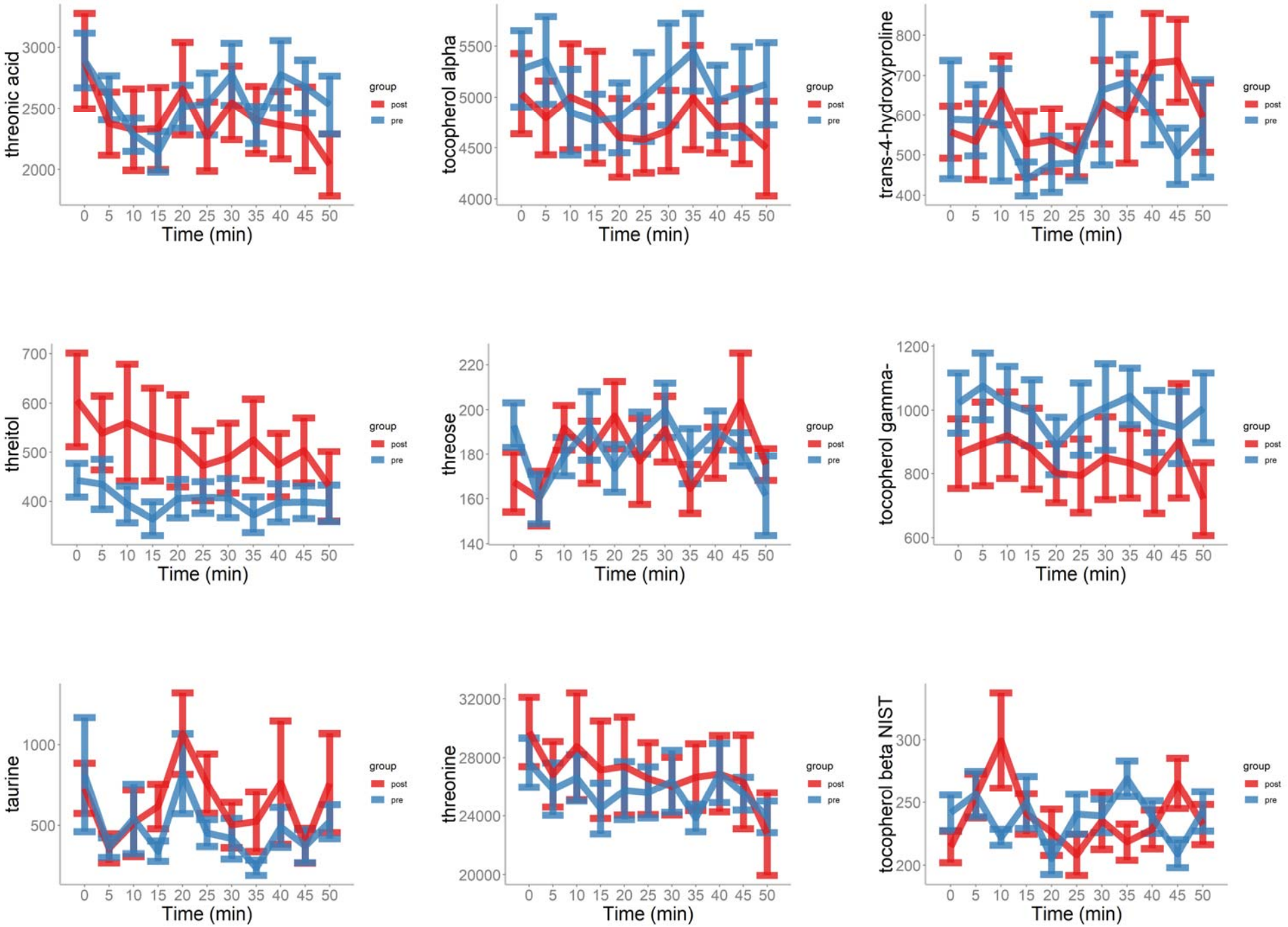
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



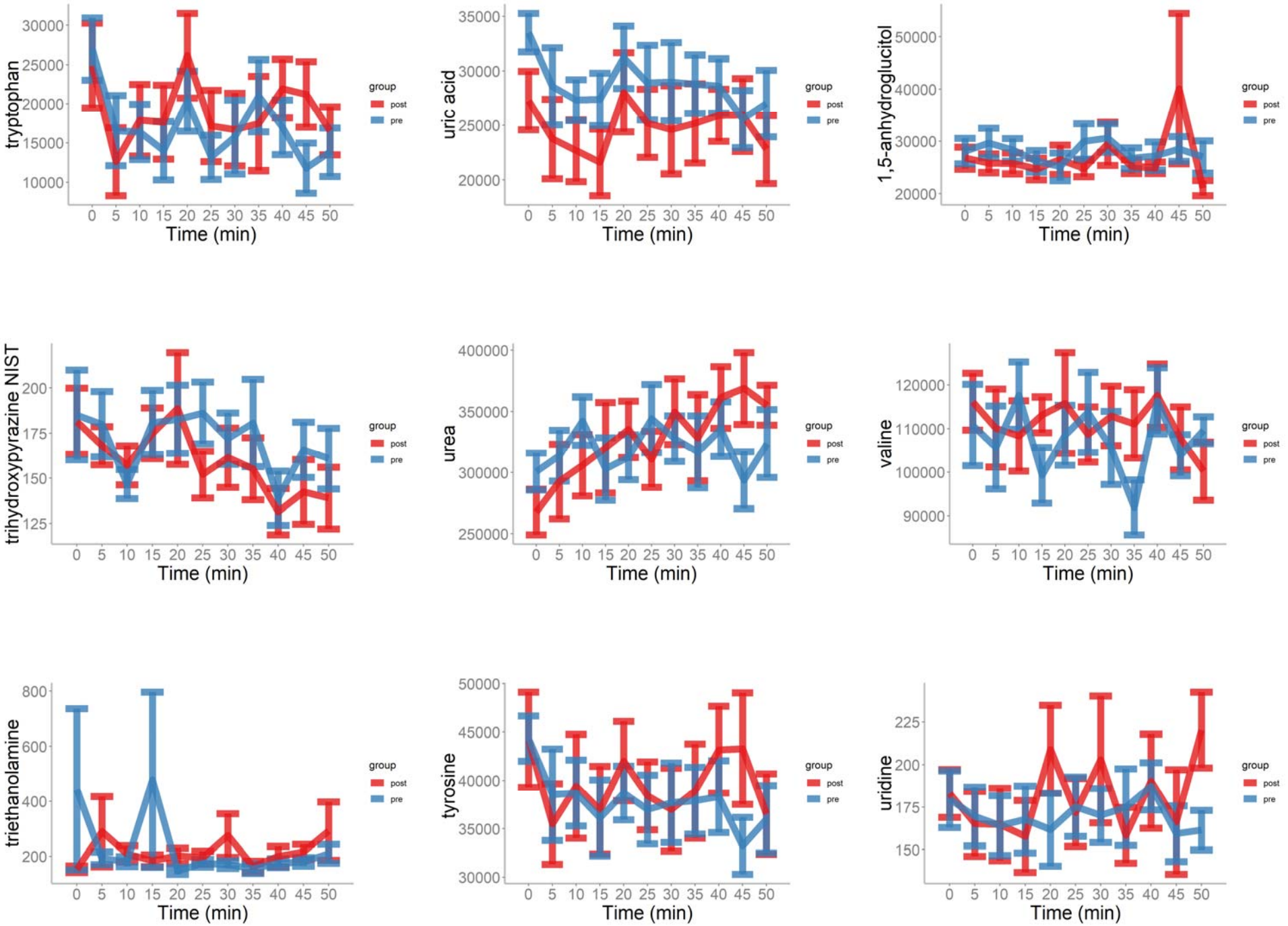
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



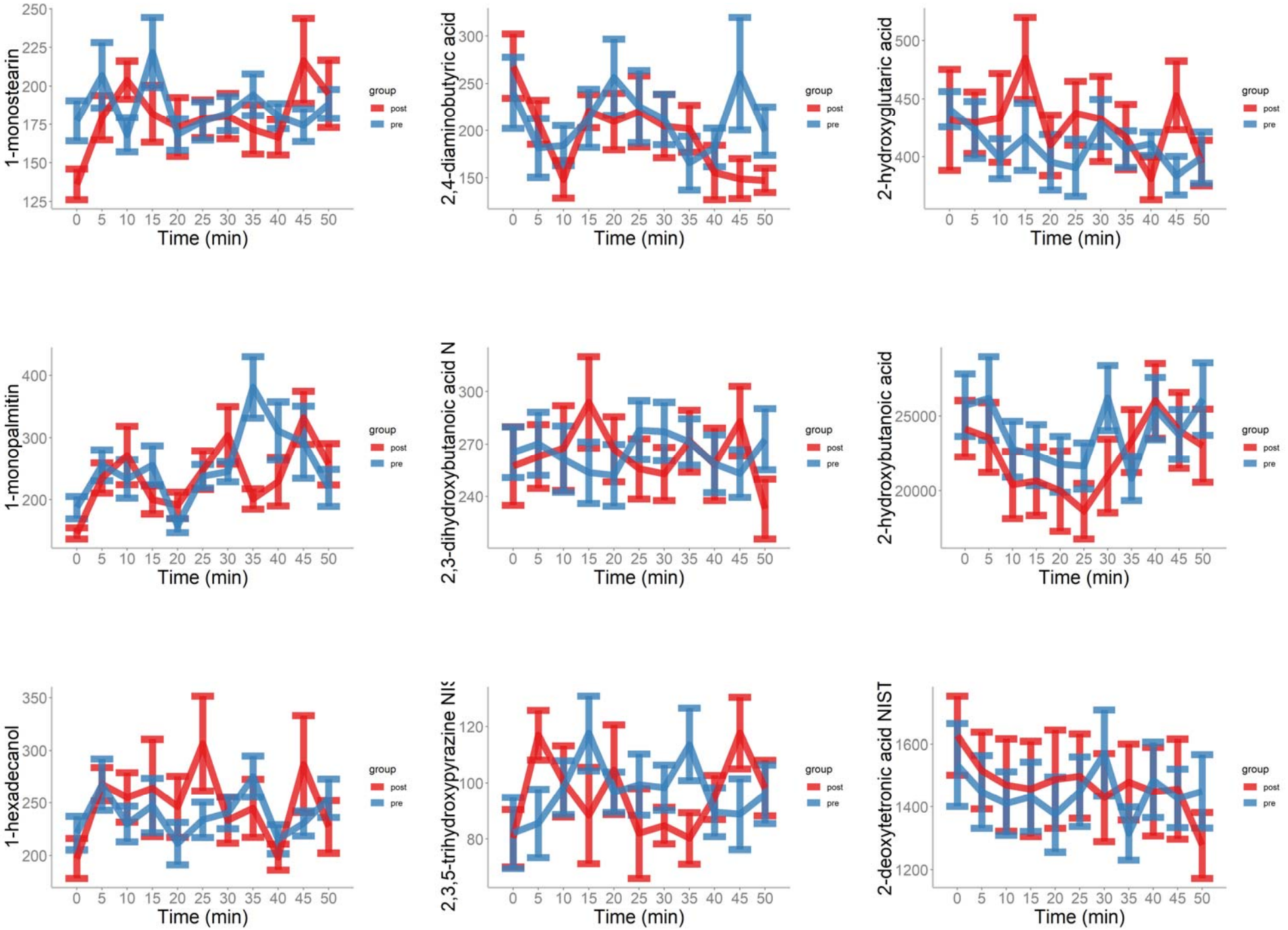
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



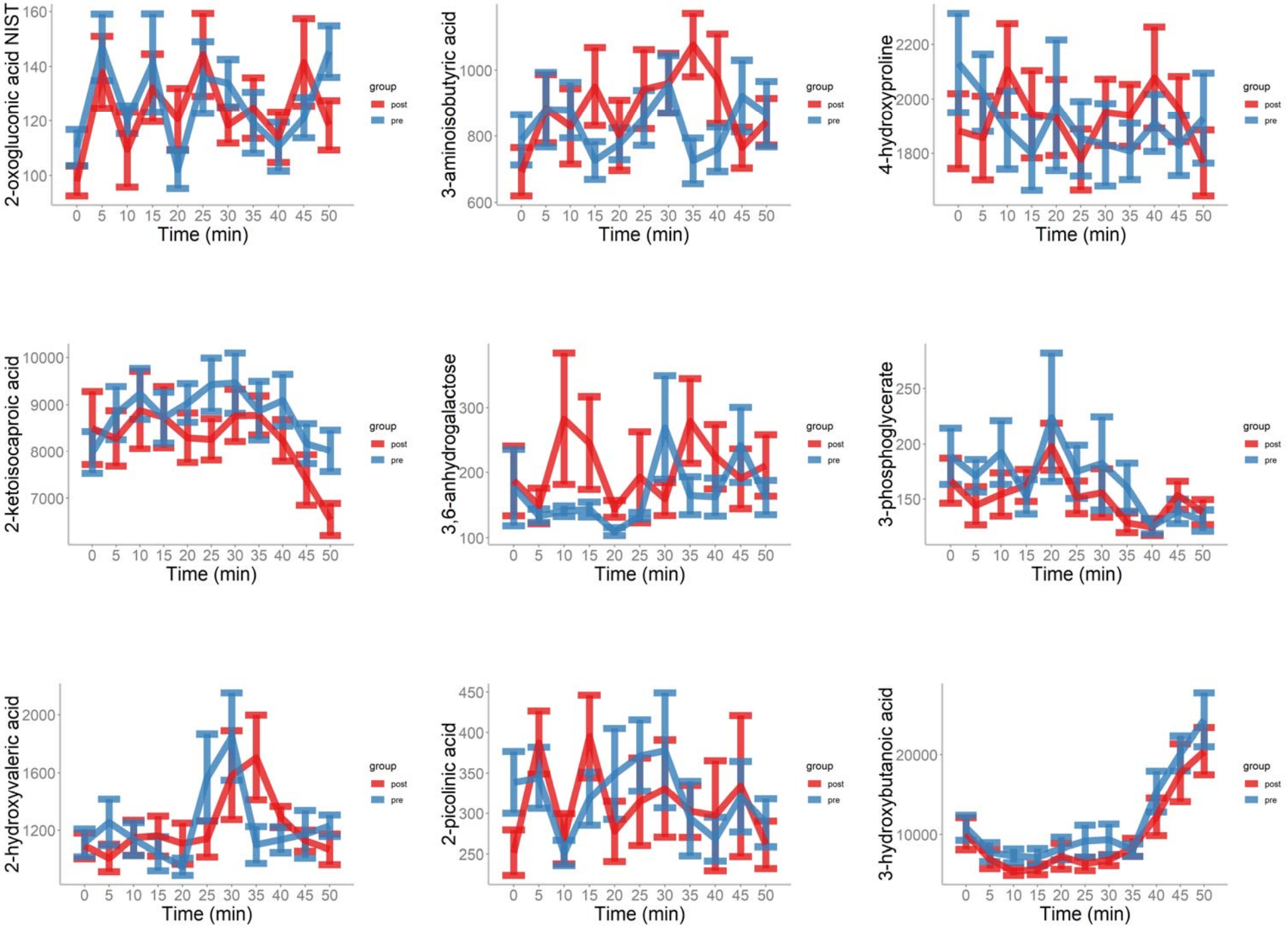
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



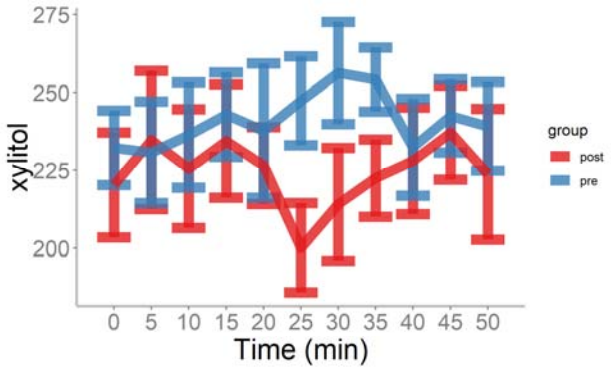
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women

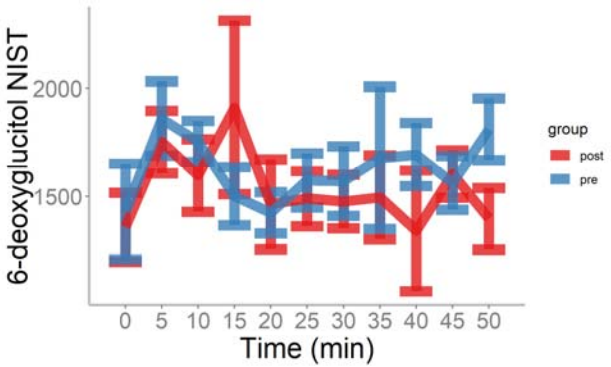


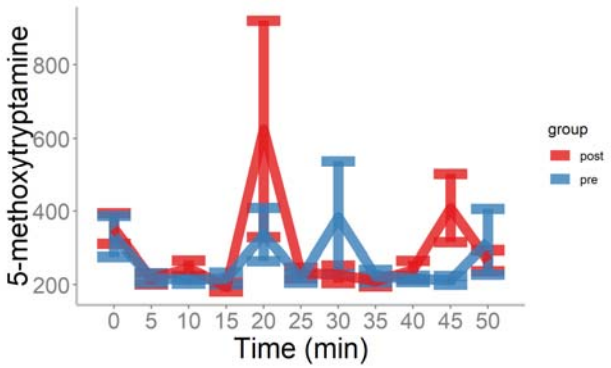
Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women



Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women

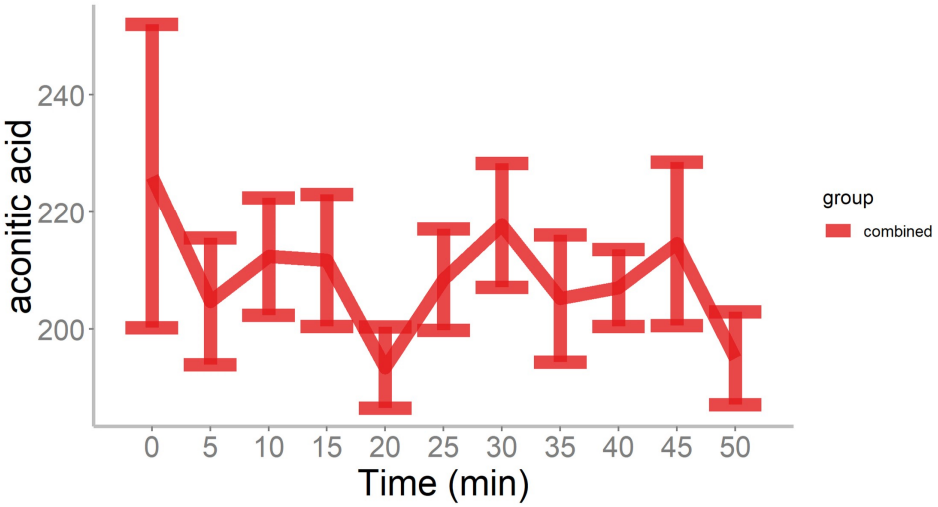


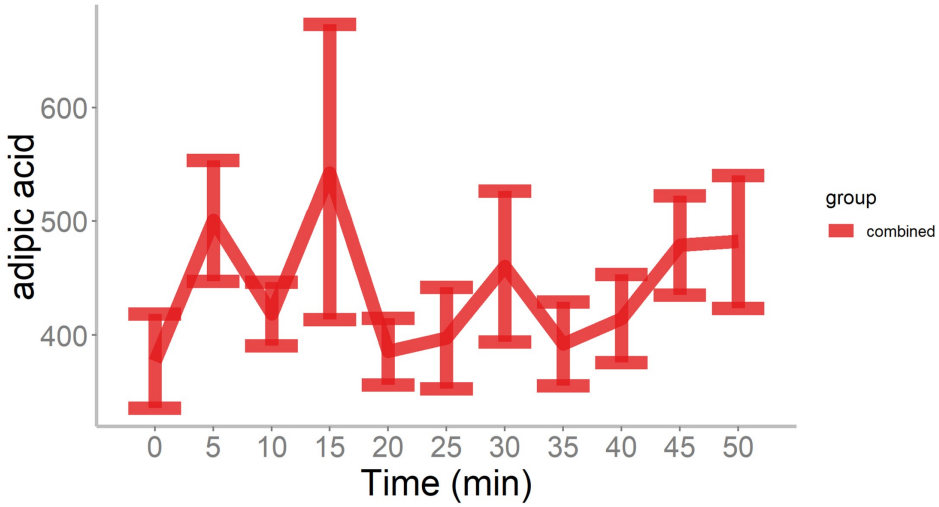




Supporting Materials 1 - Annotated metabolite concentration excursions during 30 min. fixed-workload exercise and 20 min. recovery in adult women

Supporting Materials 1B (Grapov et al.)– Individual annotated metabolite concentration excursions during 30 min. fixed-workload exercise (ergonomic cycle) and 20 min. recovery in adult obese, sedentary, insulin-resistant women, using data combined from before and after a ~14 week weight loss and fitness regimen that significantly improved metabolic health. Residuals were used from linear model for intervention (intervention-adjusted) over the measured time points (see Methods in the main paper). Concentrations are semi-quantitative and derived from metabolomics analysis and depicted here as means ± SEM based on quantifier peak ion heights.


aconitic acid
240
220
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


adipic acid
600
500
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
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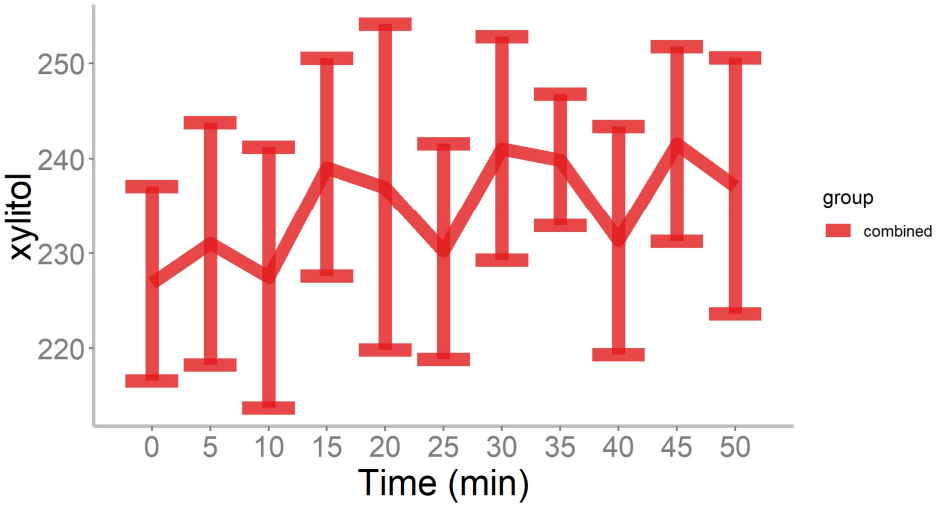
xylitol
250
240
230
220
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Time (min)
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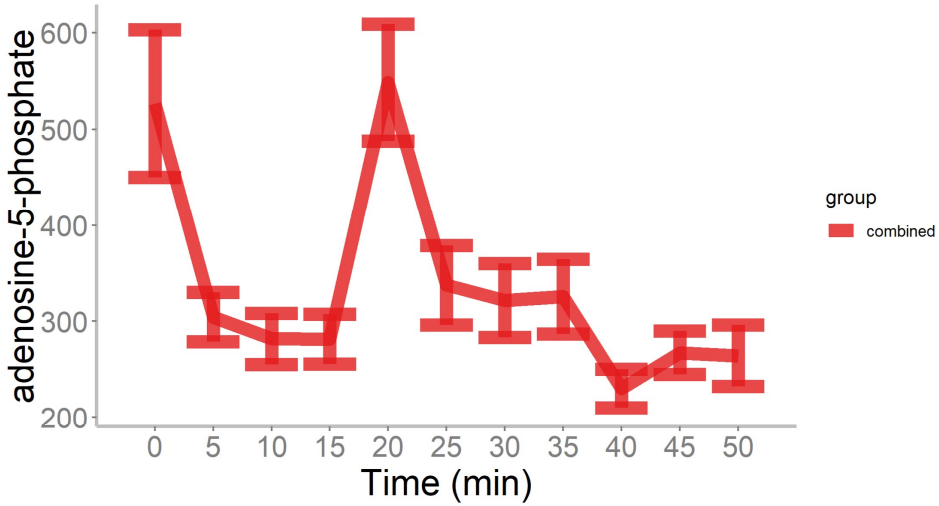
adenosine-5-phosphate
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500
400
300
200
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Time (min)
group
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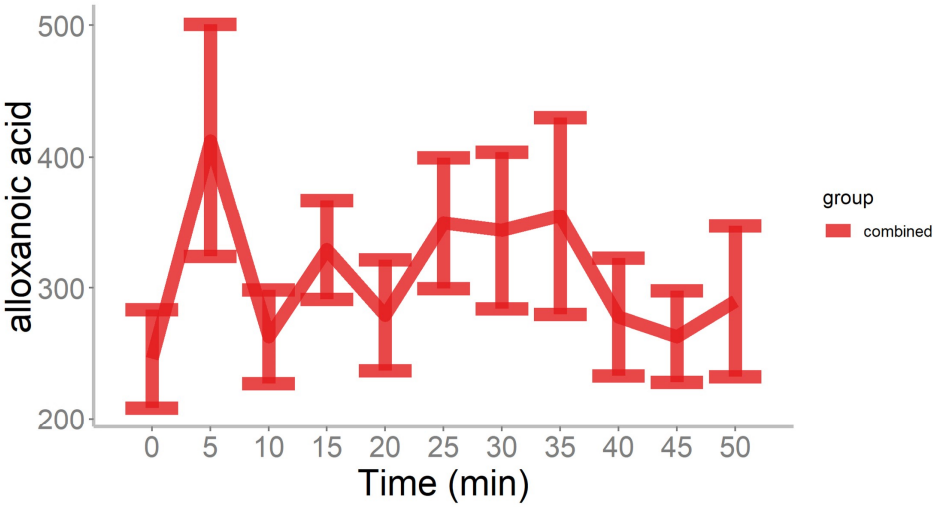
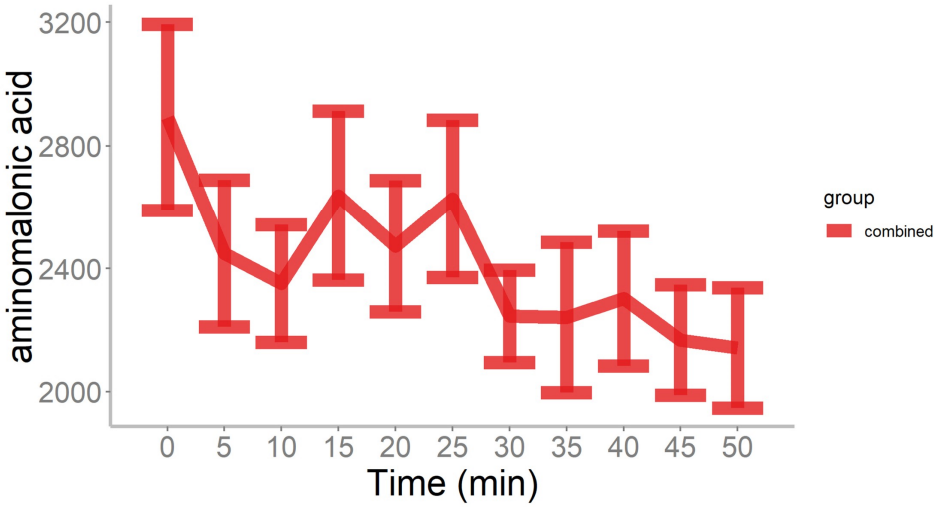

alloxanoic acid
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


aminomalonic acid
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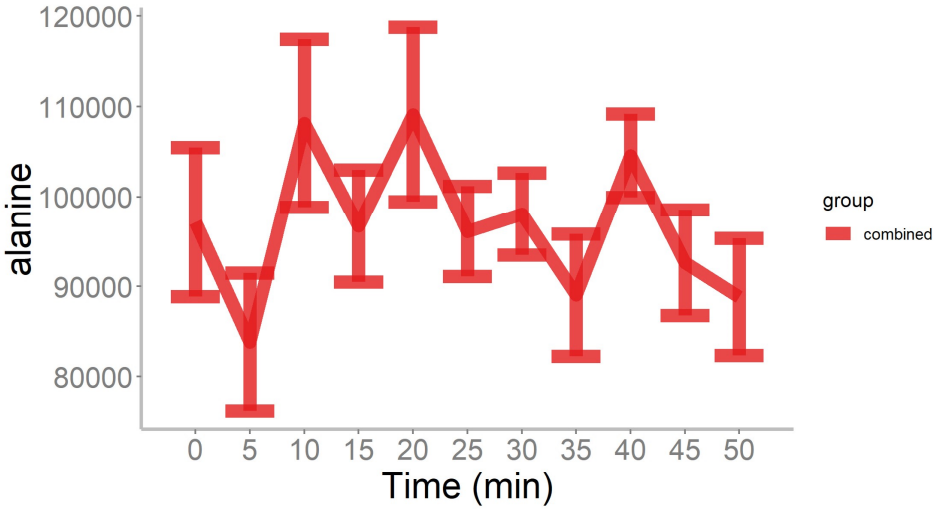
2800
2400
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


alanine
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100000
90000
80000
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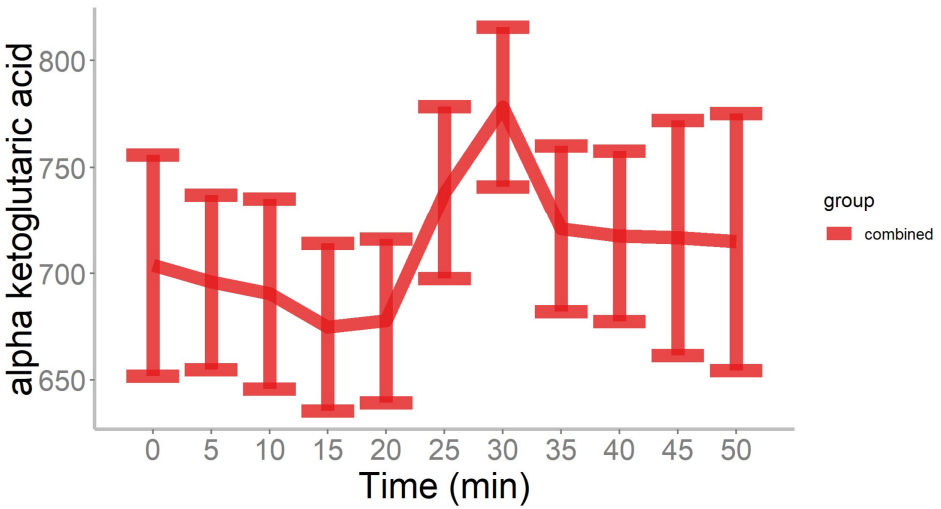
Time (min)
group
combined


alpha ketoglutaric acid
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750
700
650
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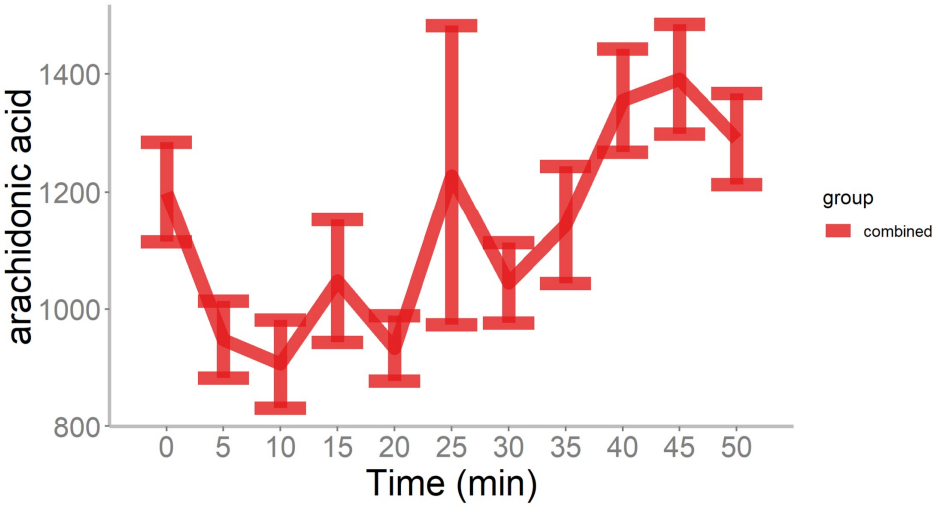
Time (min)
group
combined


arachidonic acid
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1200
1000
800
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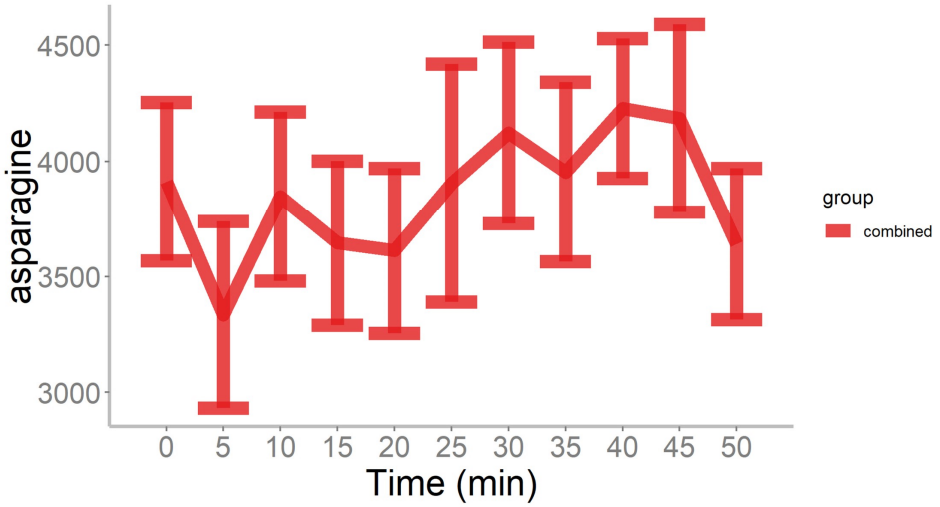
Time (min)
group
combined


asparagine
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4000
3500
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Time (min)
group
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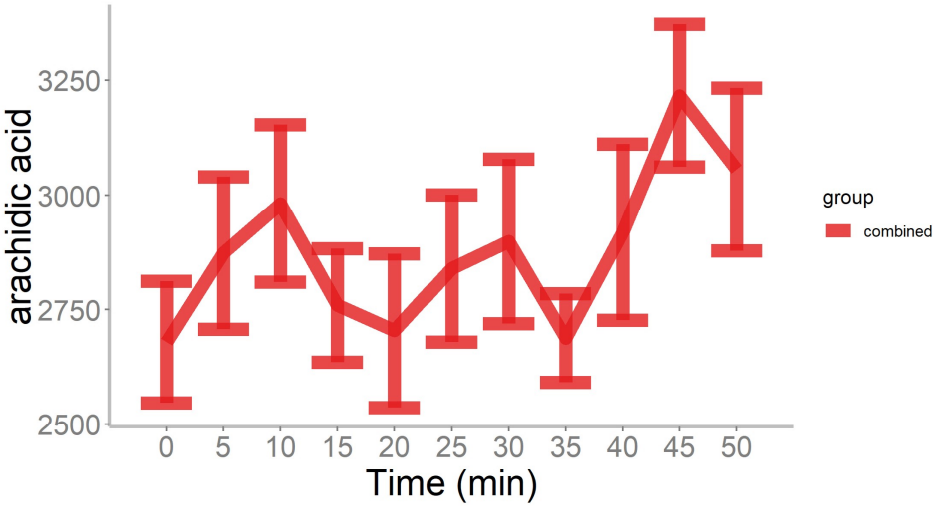
arachidic acid
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2750
2500
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Time (min)
group
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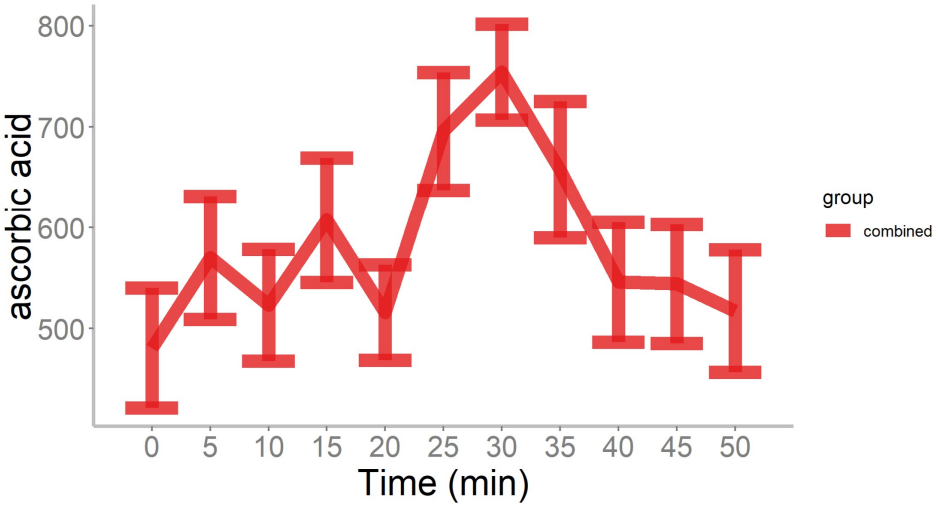
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800
700
600
500
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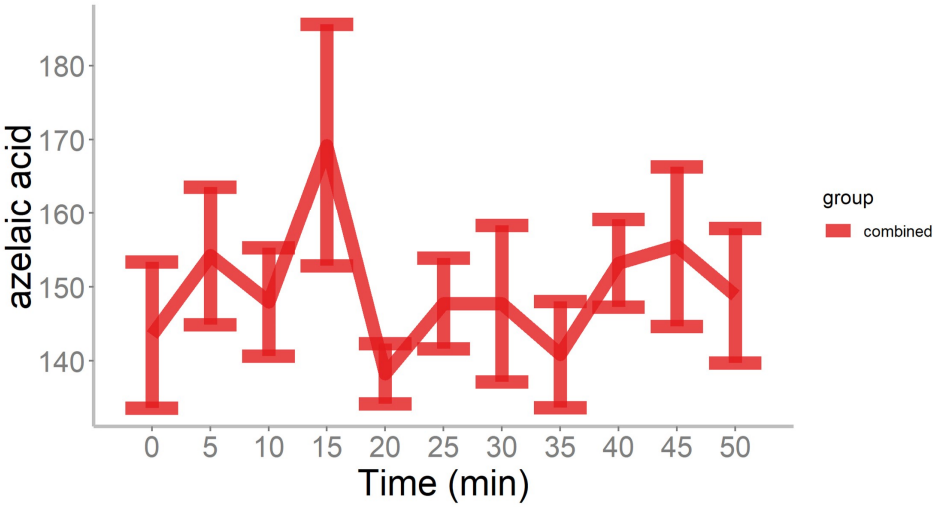
Time (min)
group
combined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170
160
150
140
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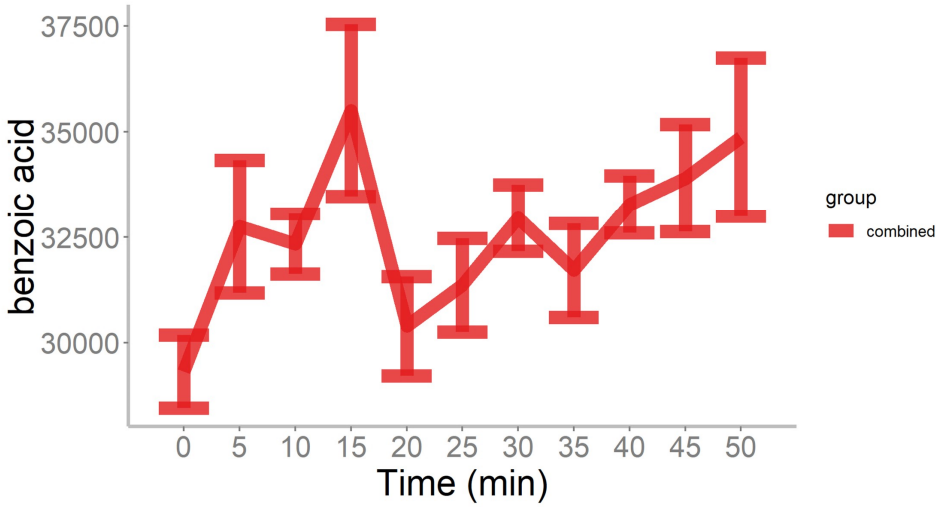
Time (min)
group
combined


benzoic acid
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35000
32500
30000
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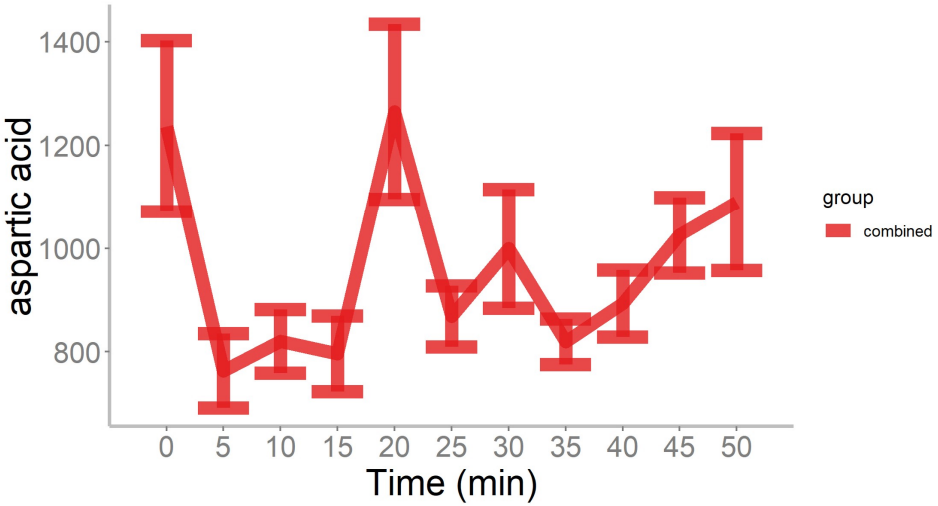
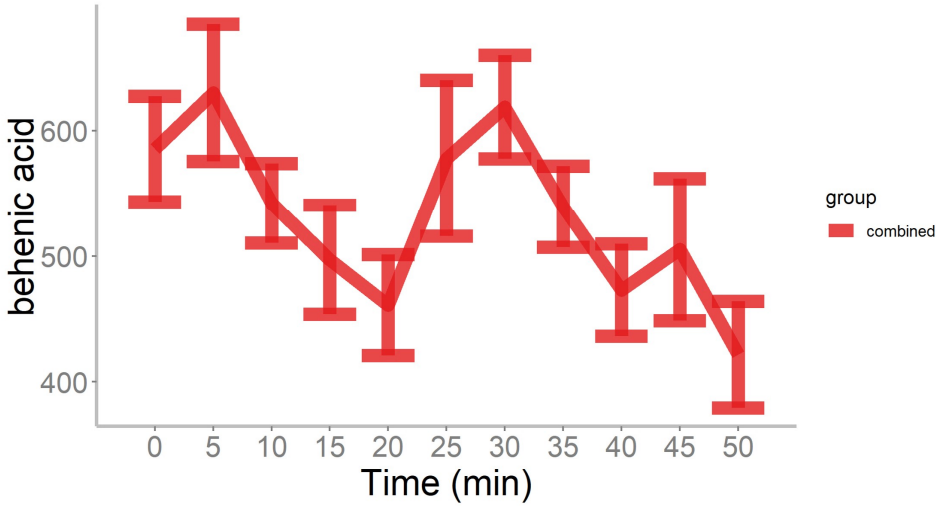
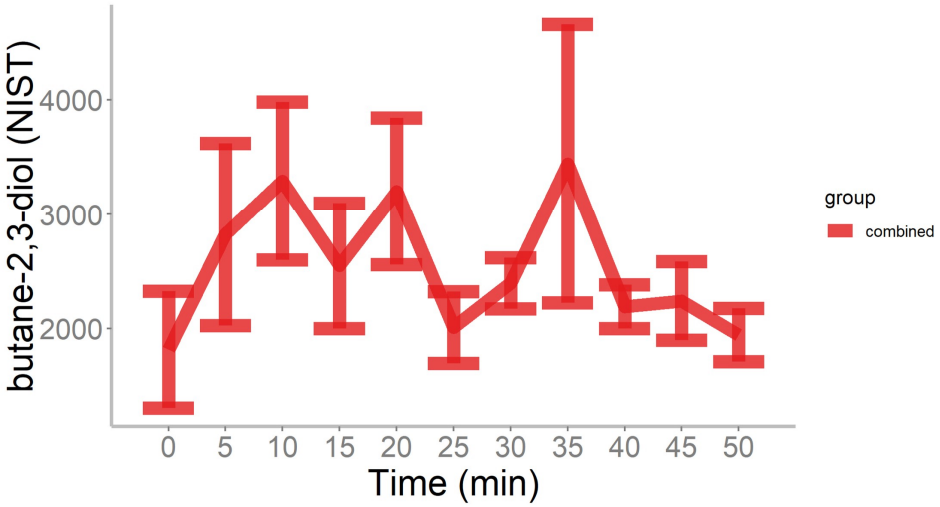
Time (min)
group
combined


aspartic acid
1400
1200
1000
800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


behenic acid
600
500
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


butane-2,3-diol (NIST)
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3000
2000
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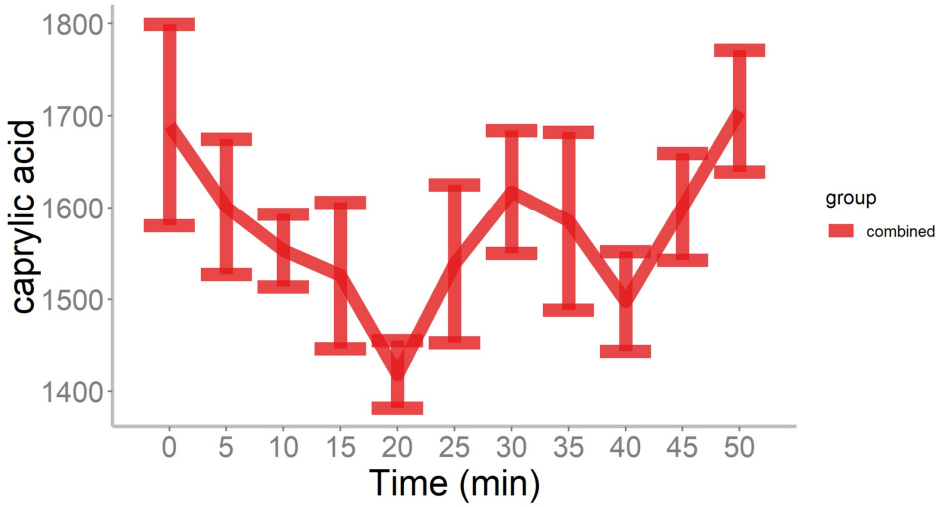
Time (min)
group
combined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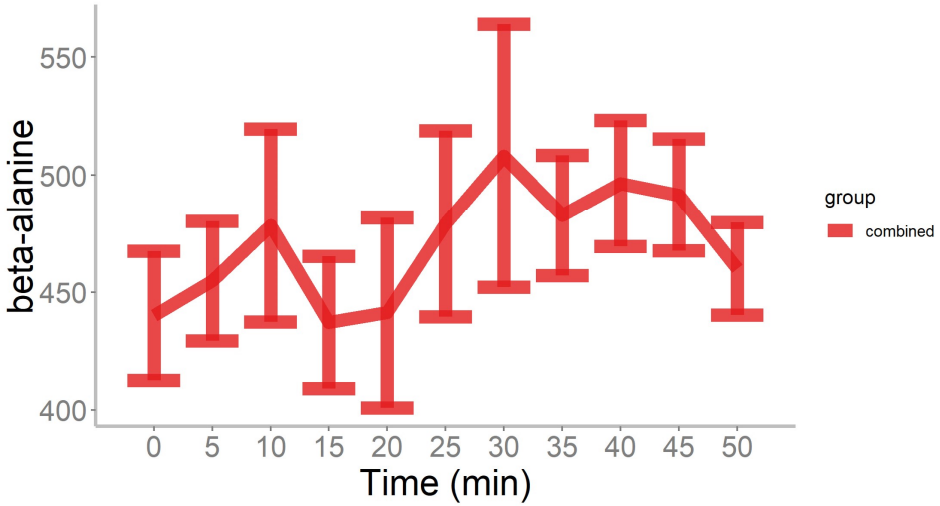
1700
1600
1500
1400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


beta-alanine
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500
450
400
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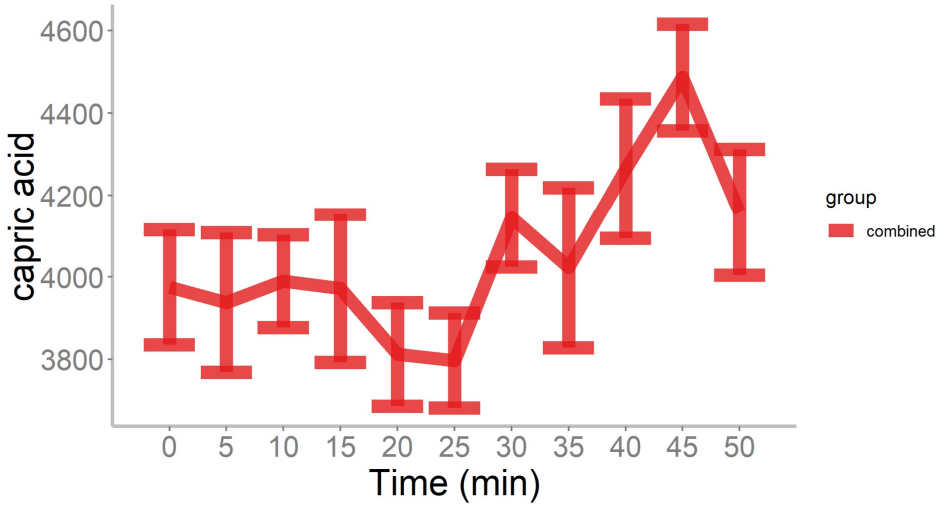
Time (min)
group
combined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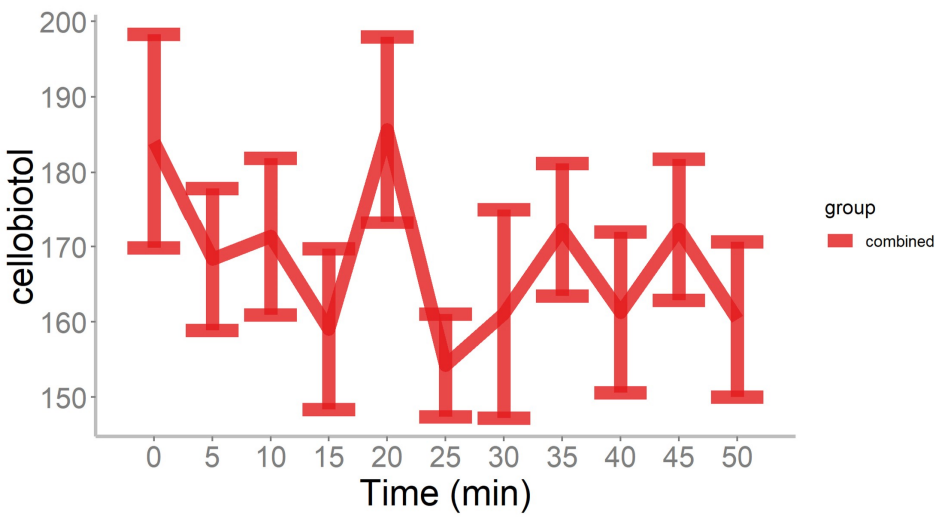
Time (min)
group
combined


cellobiotol
200
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180
170
160
150
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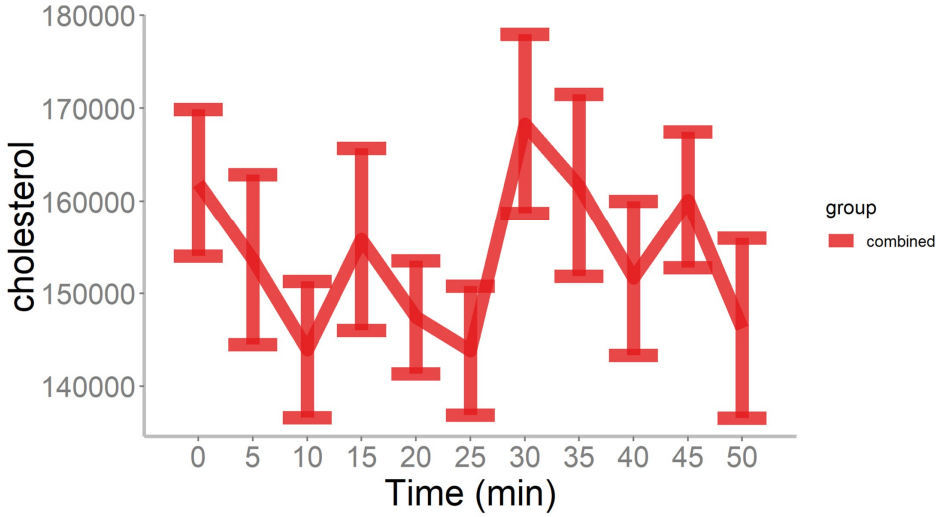
Time (min)
group
combined


cholesterol
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160000
150000
140000
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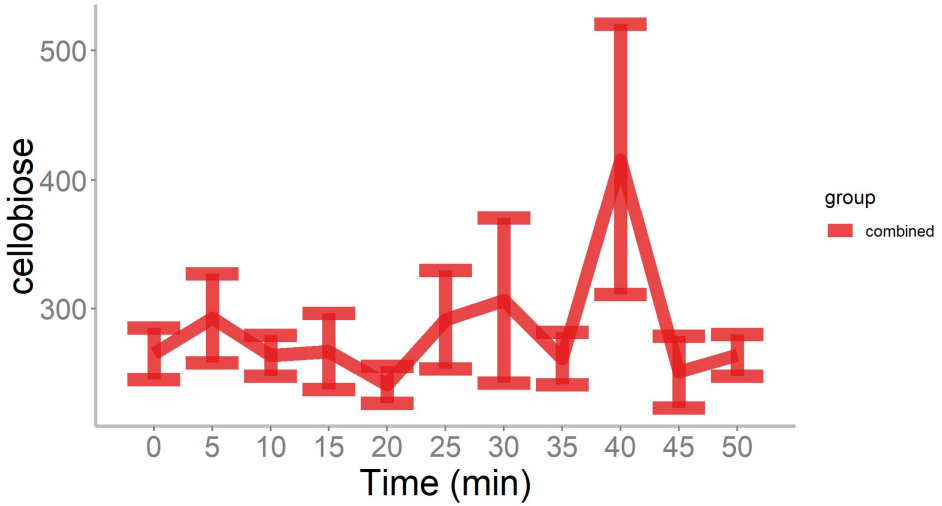
Time (min)
group
combined


cellobiose
500
400
300
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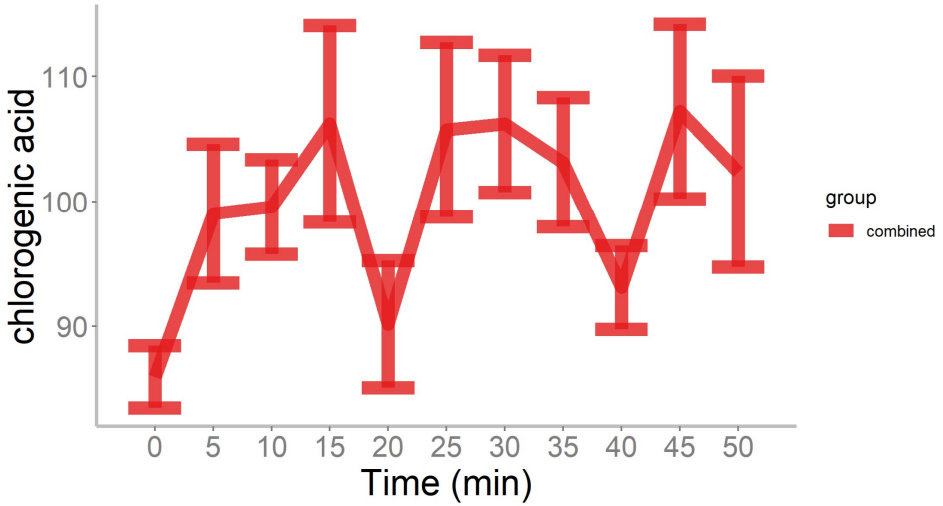
Time (min)
group
combined


chlorogenic acid
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100
90
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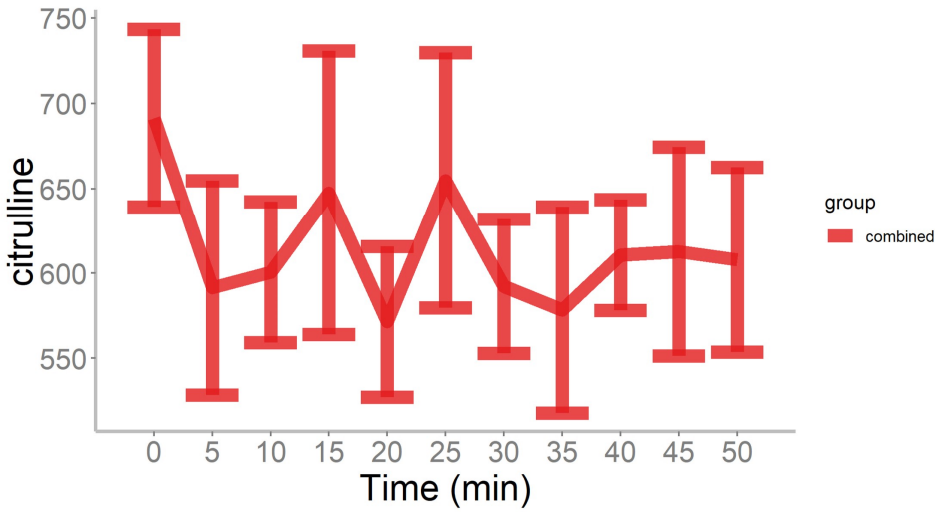
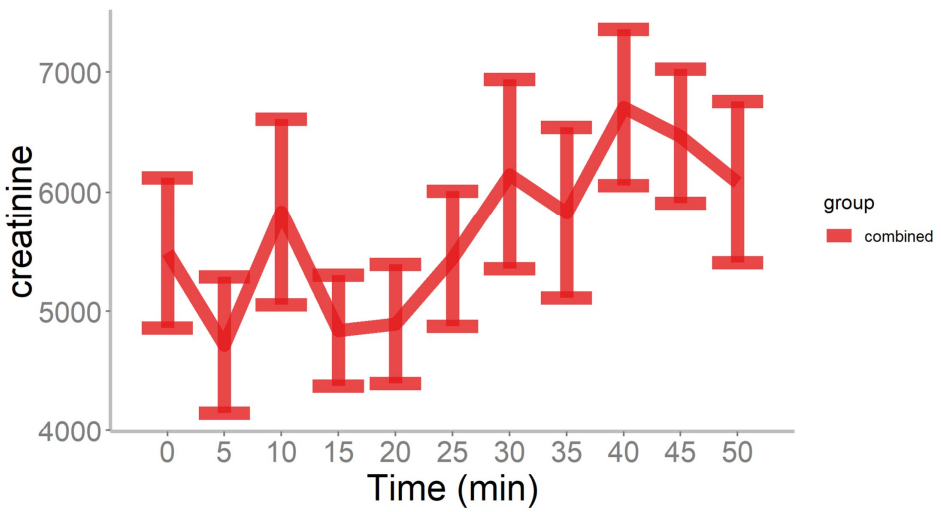
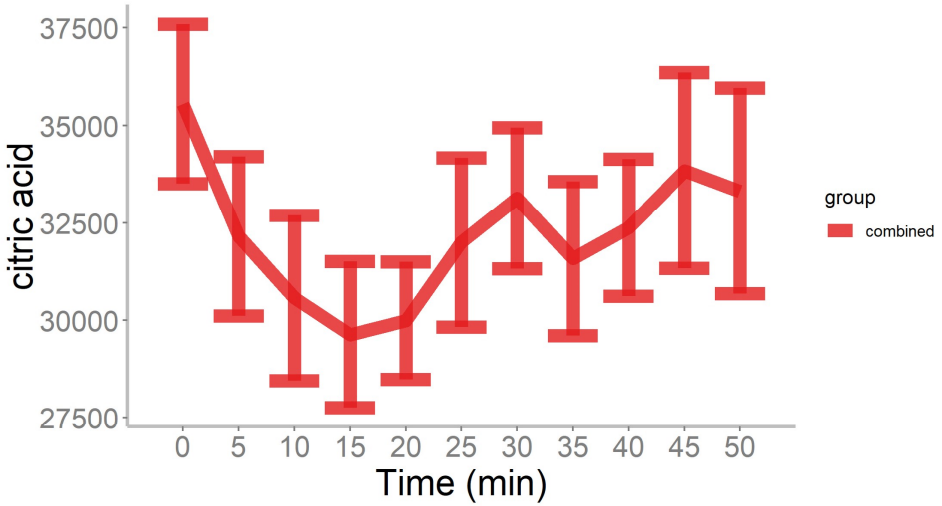
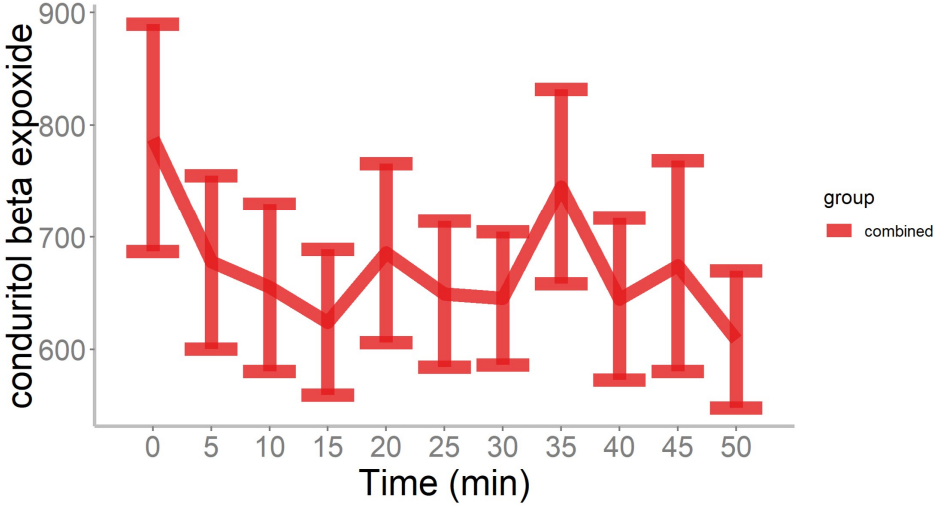
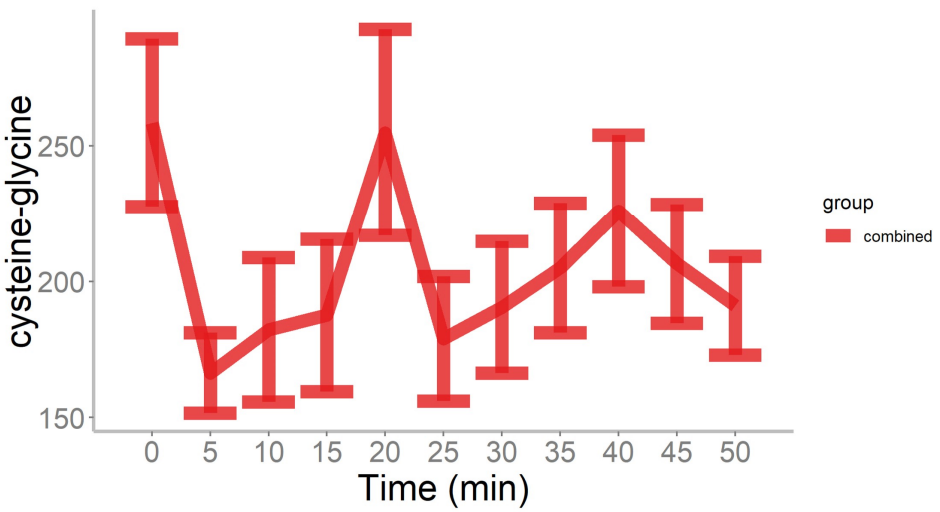
Time (min)
group
combined


citrulline
750
700
650
600
550
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


creatinine
7000
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


citric acid
37500
35000
32500
30000
27500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


conduritol beta expoxide
900
800
700
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


cysteine-glycine
150
200
250
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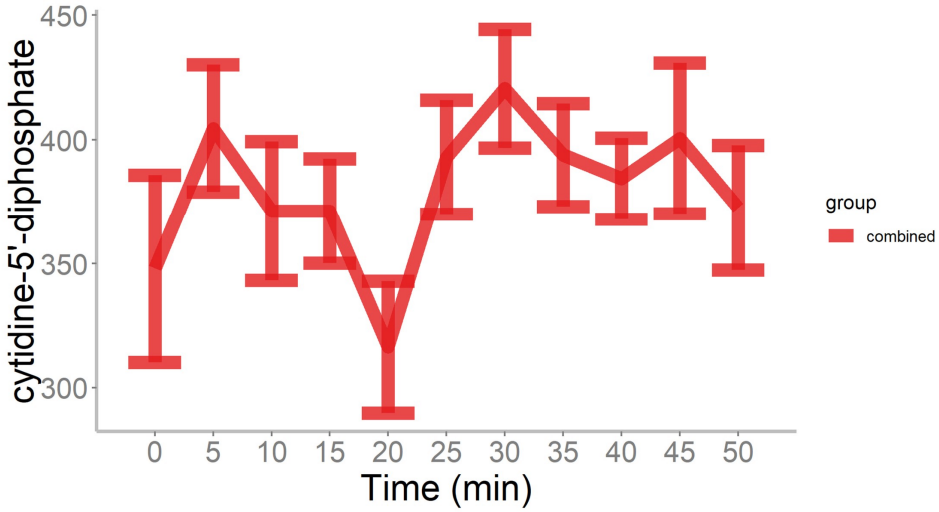
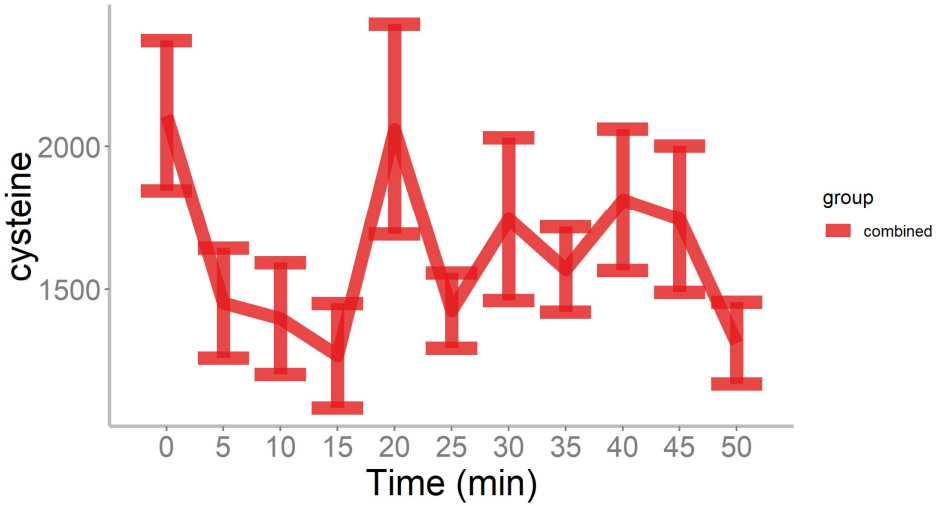
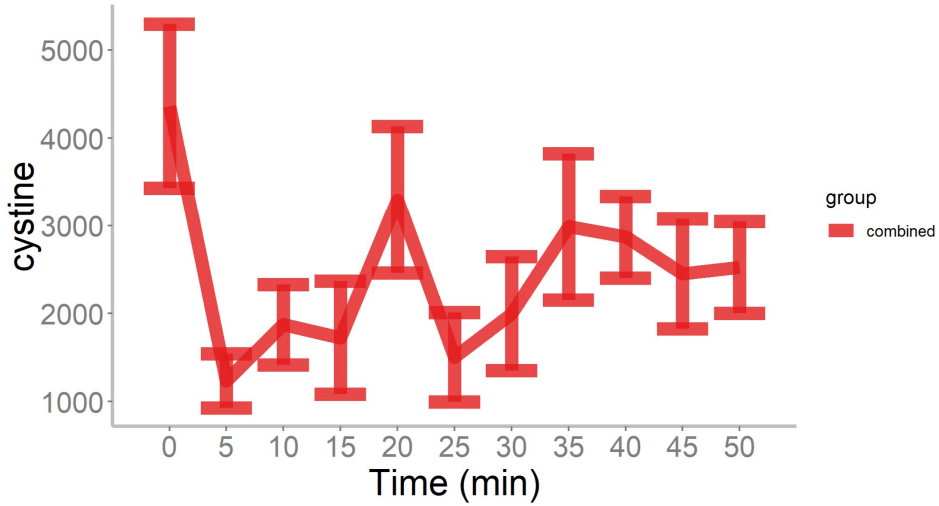
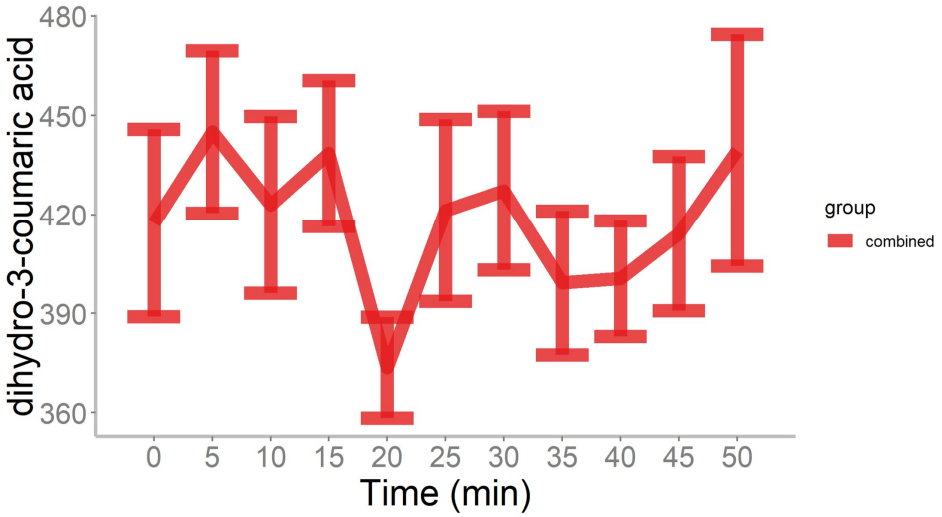
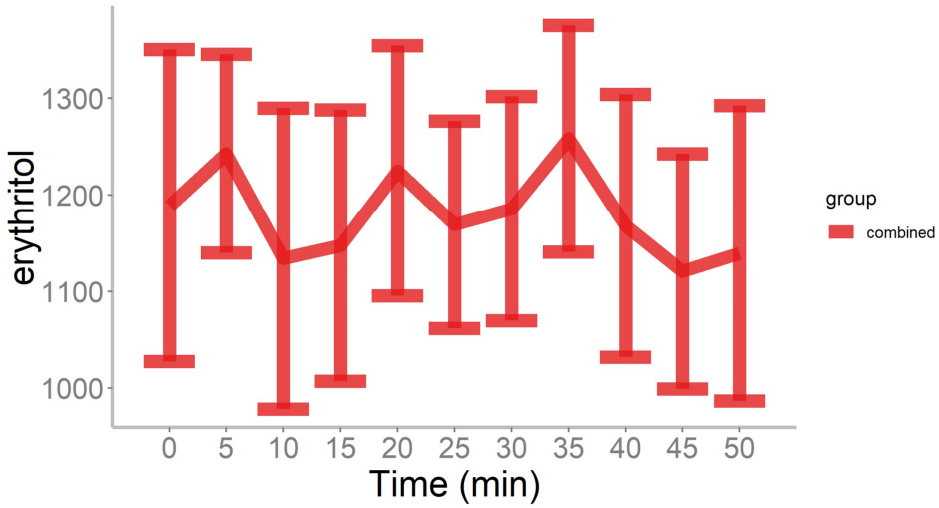
Time (min)
group
combined

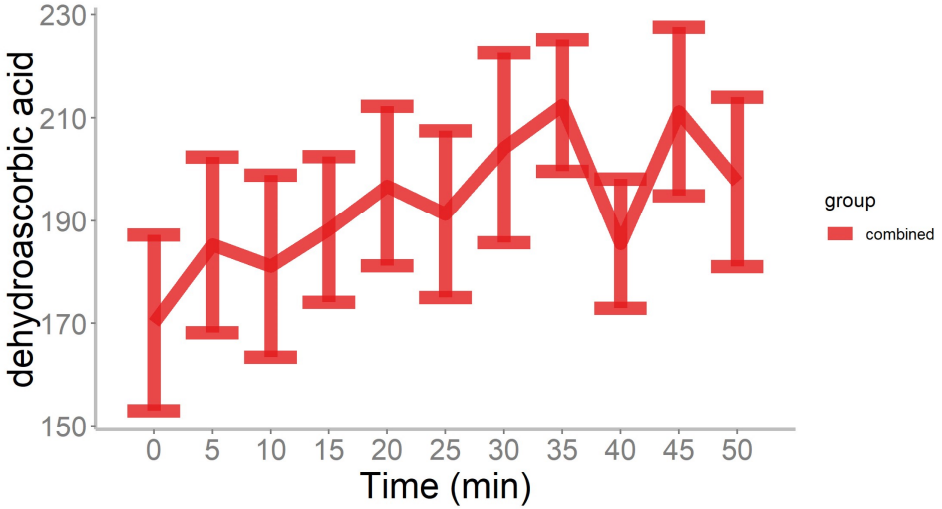

cytidine-5'-diphosphate
300
350
400
450
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

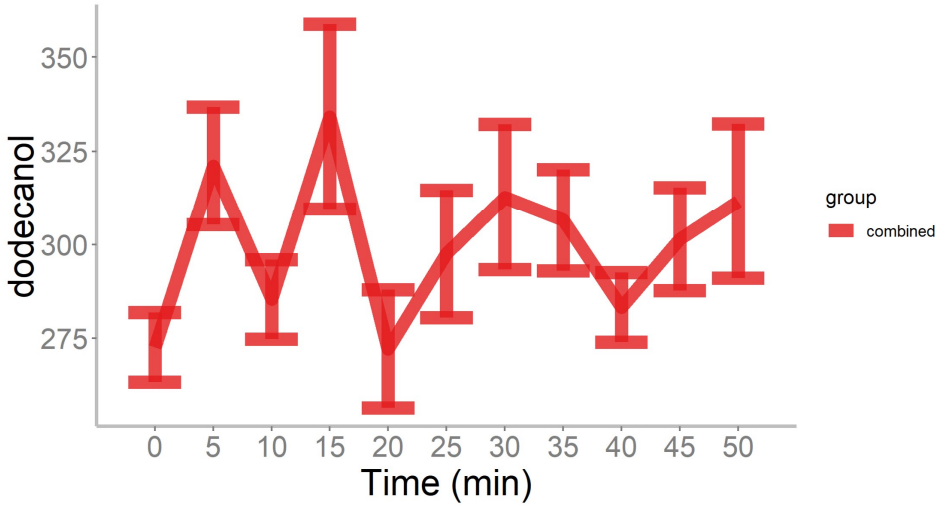

cysteine
1500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

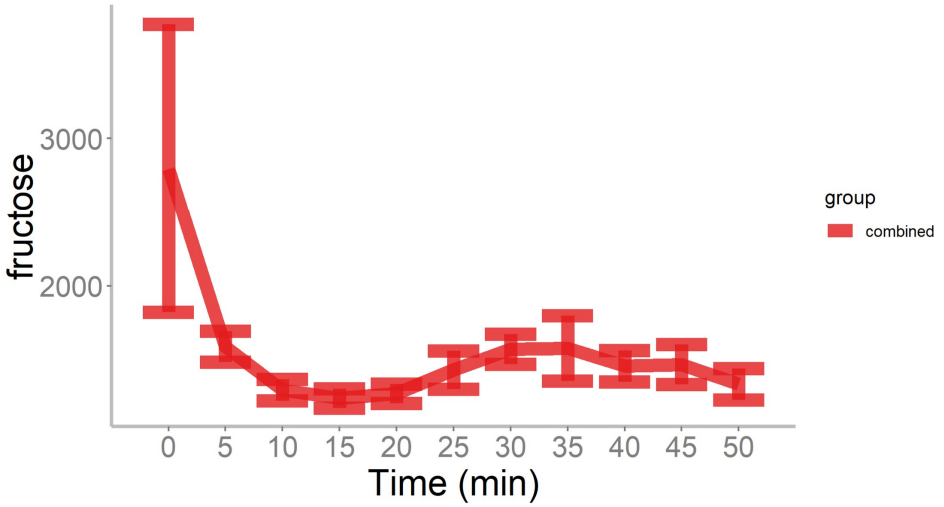

cystine
1000
2000
3000
4000
5000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

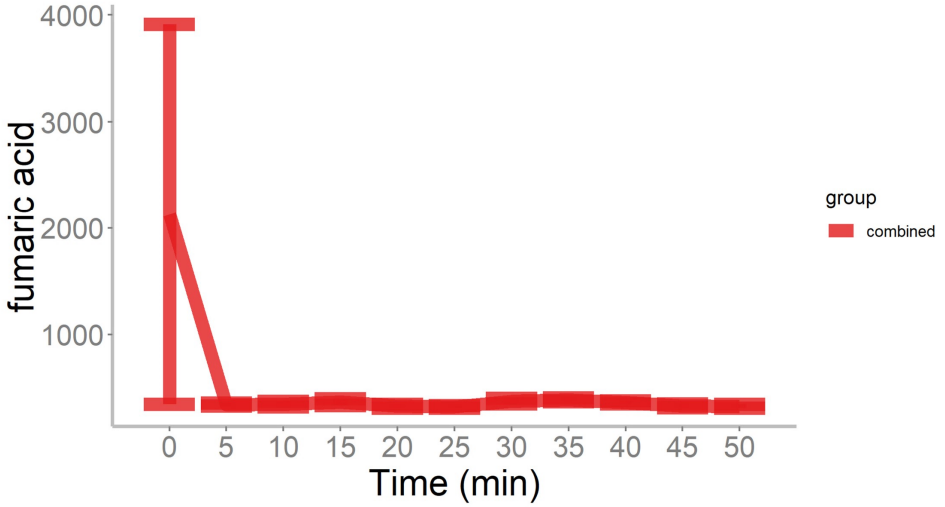

dihydro-3-coumaric acid
480
450
420
390
360
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

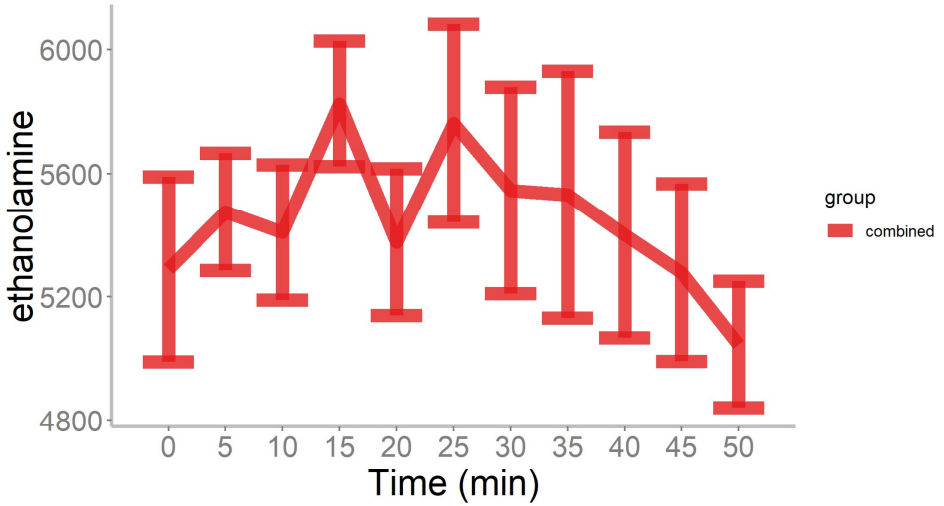

erythritol
1300
1200
1100
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

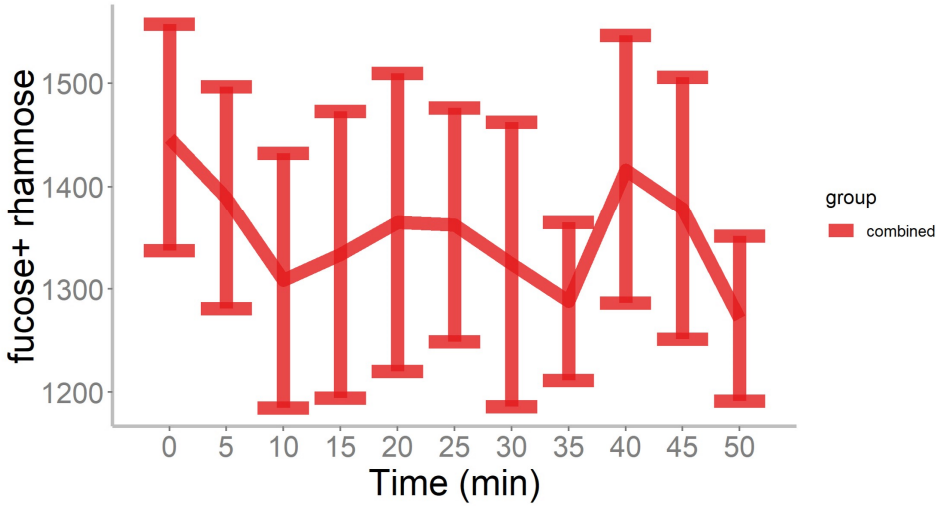

dehydroascorbic acid
230
210
190
170
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

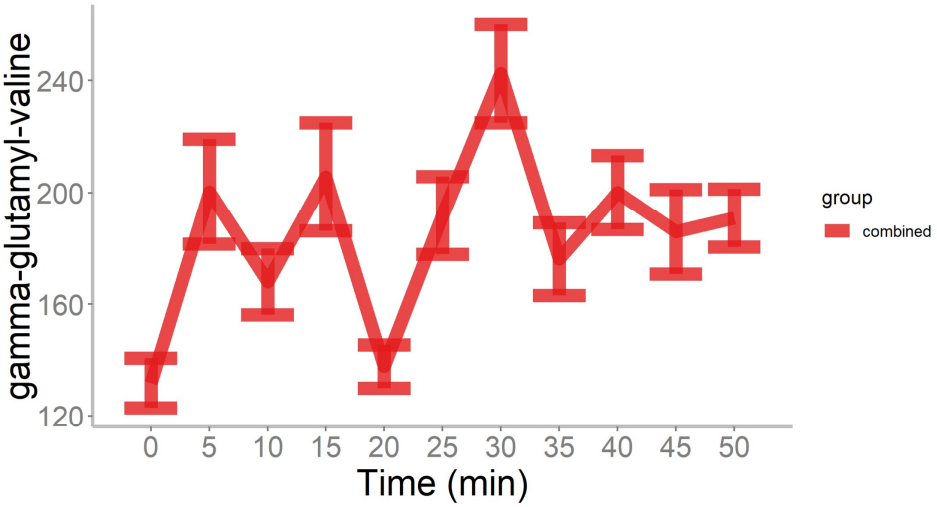

dodecanol
350
325
300
275
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

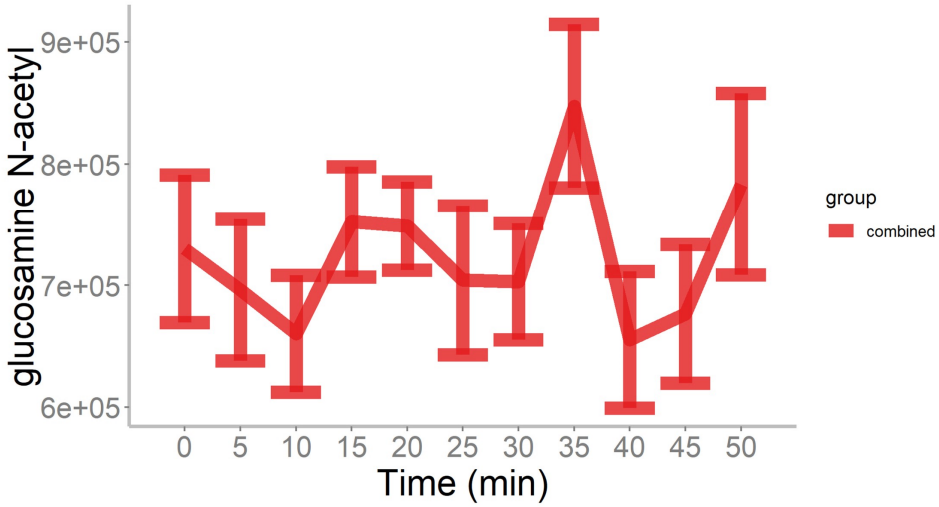

fructose
3000
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

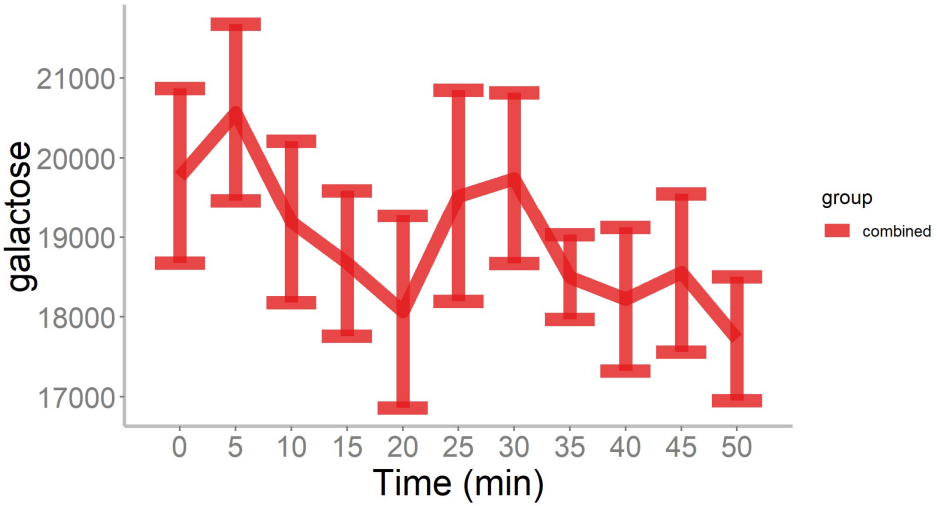

fumaric acid
4000
3000
2000
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

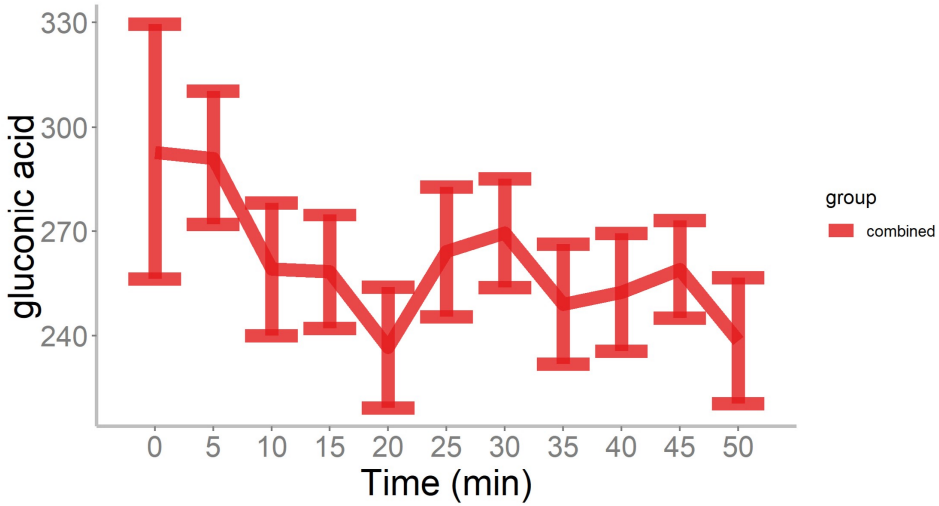

ethanolamine
6000
5600
5200
4800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

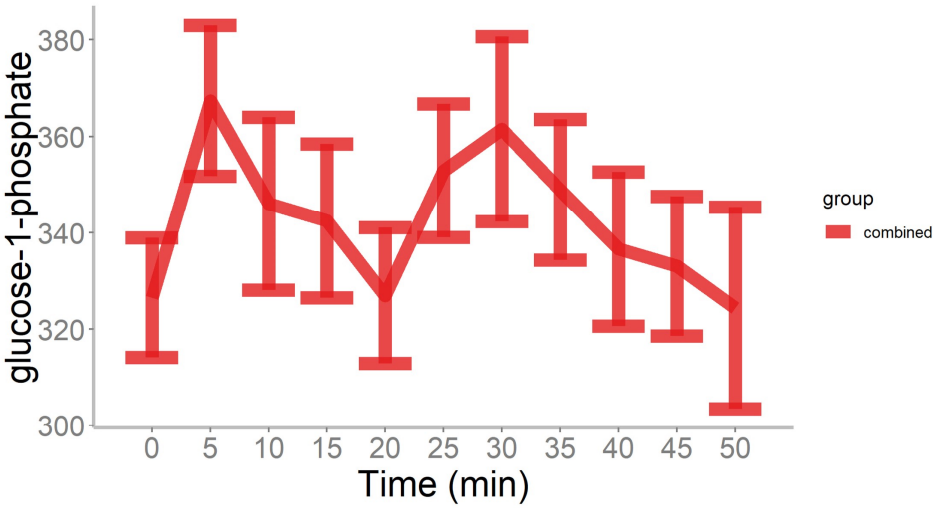

fucose+ rhamnose
1500
1400
1300
1200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

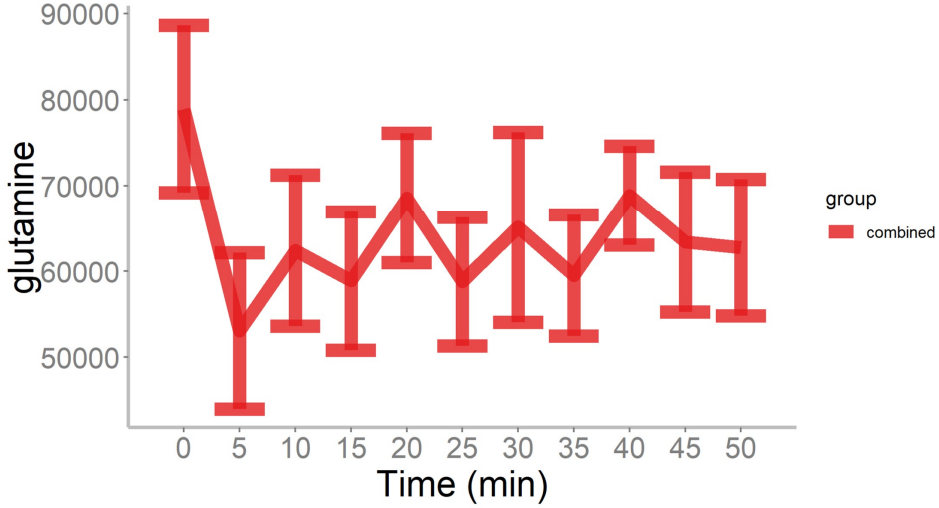

gamma-glutamyl-valine
240
200
160
120
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

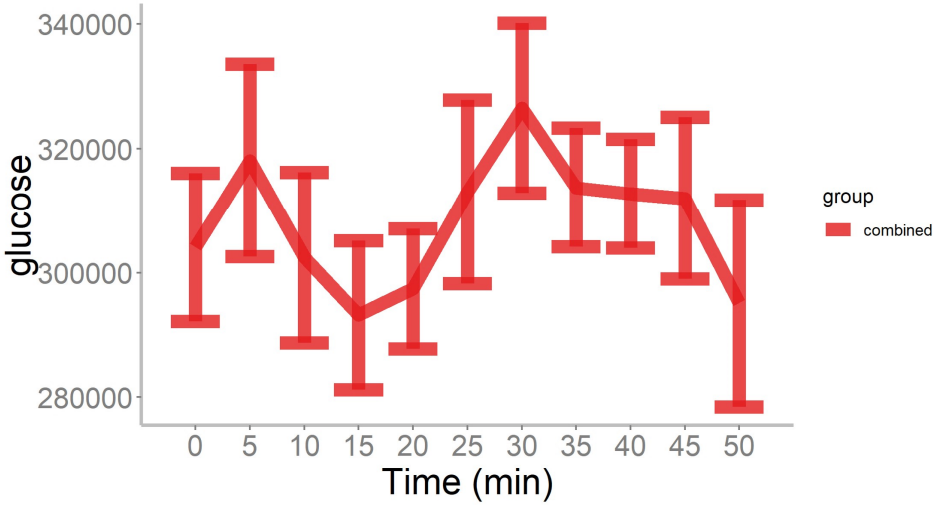

glucosamine N-acetyl
9e+05
8e+05
7e+05
6e+05
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

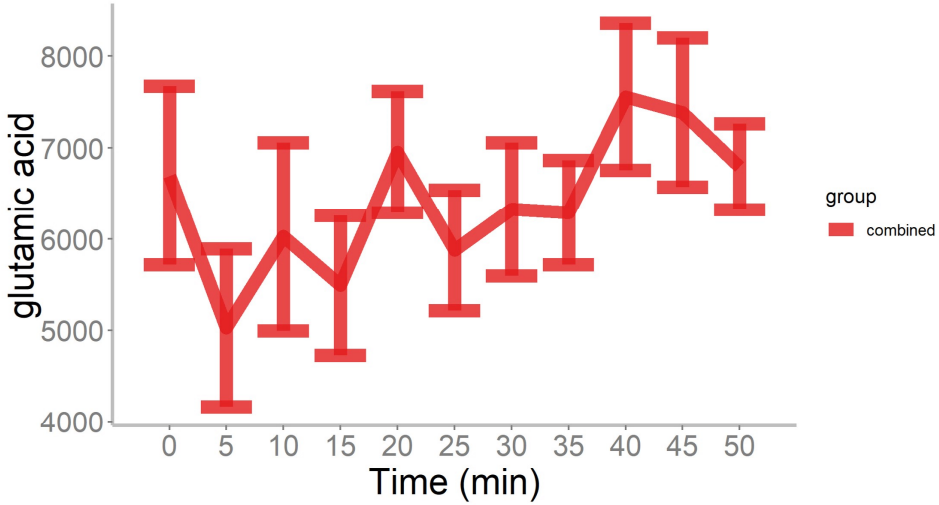

galactose
21000
20000
19000
18000
17000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

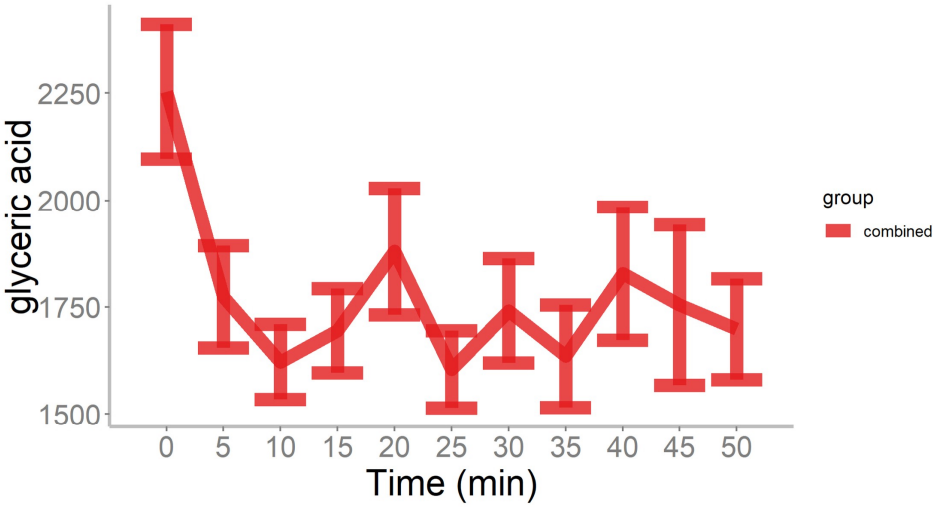

gluconic acid
330
300
270
240
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

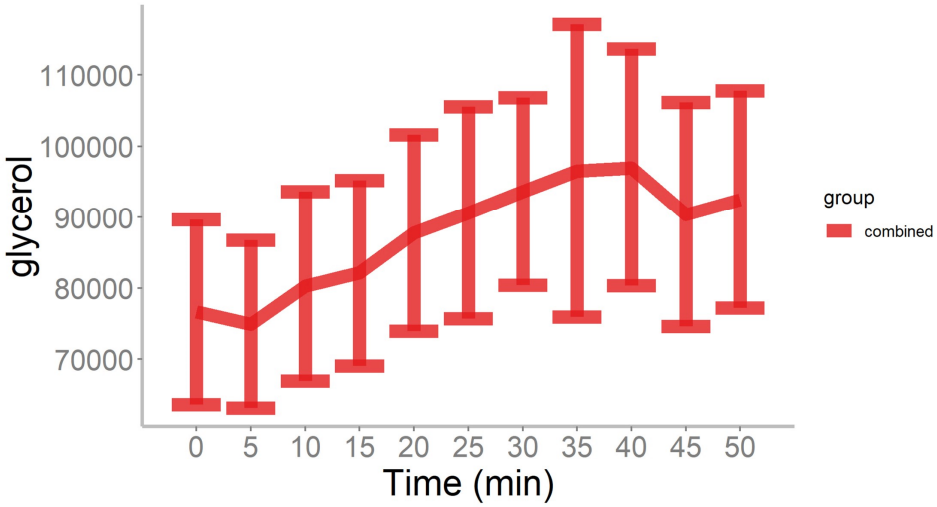

glucose-1-phosphate
380
360
340
320
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

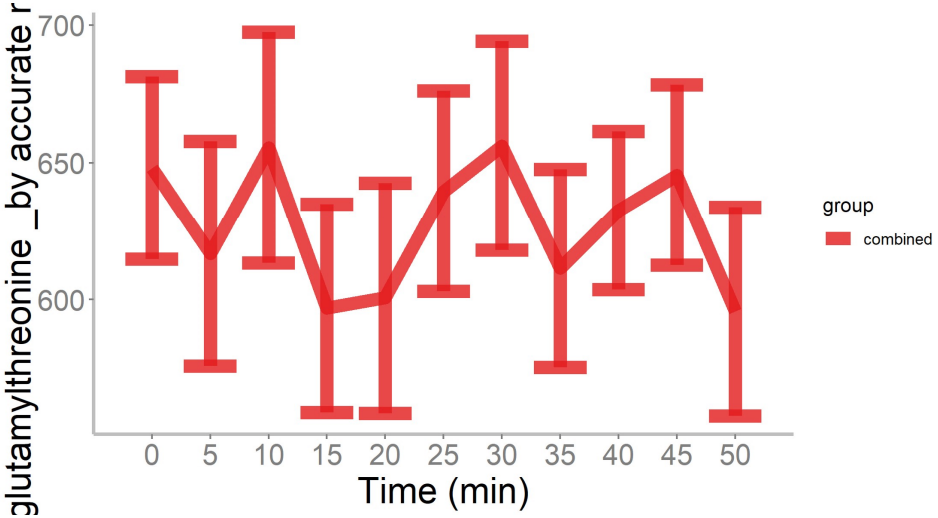

glutamine
90000
80000
70000
60000
50000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

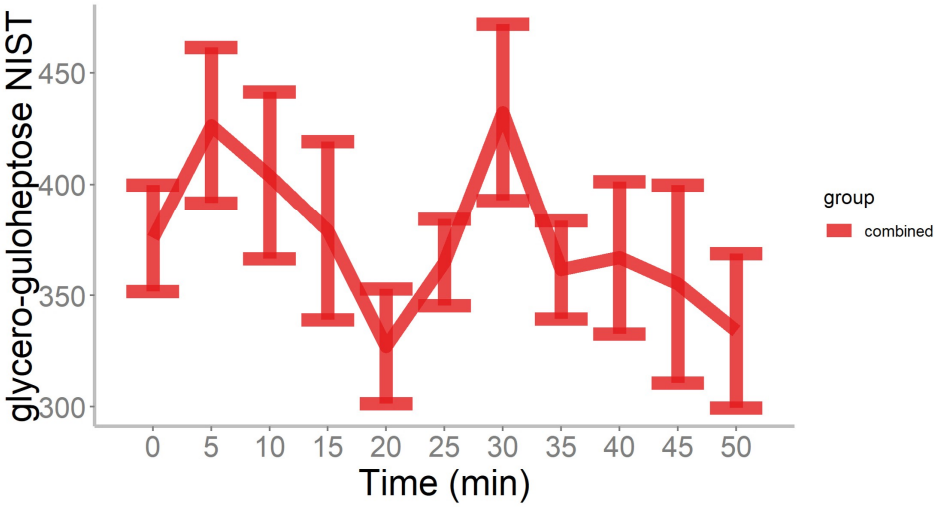

glucose
340000
320000
300000
280000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

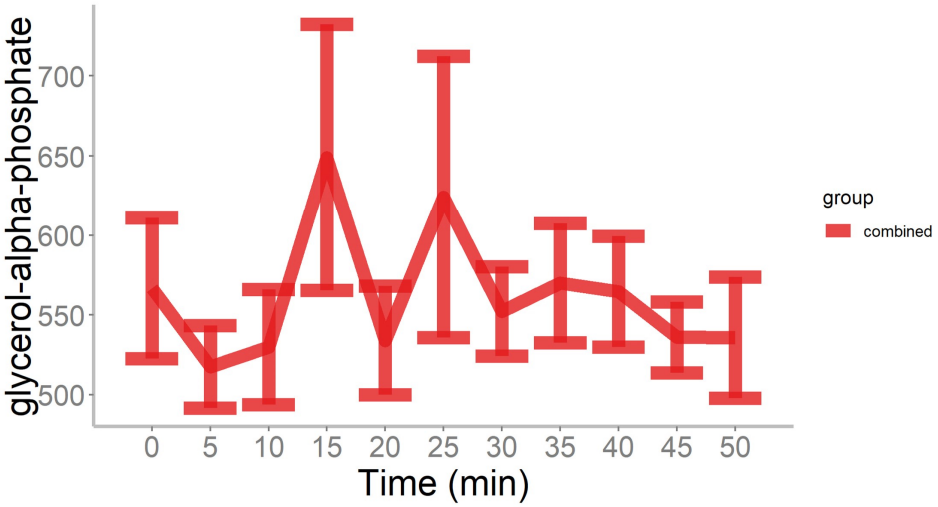

glutamic acid
8000
7000
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

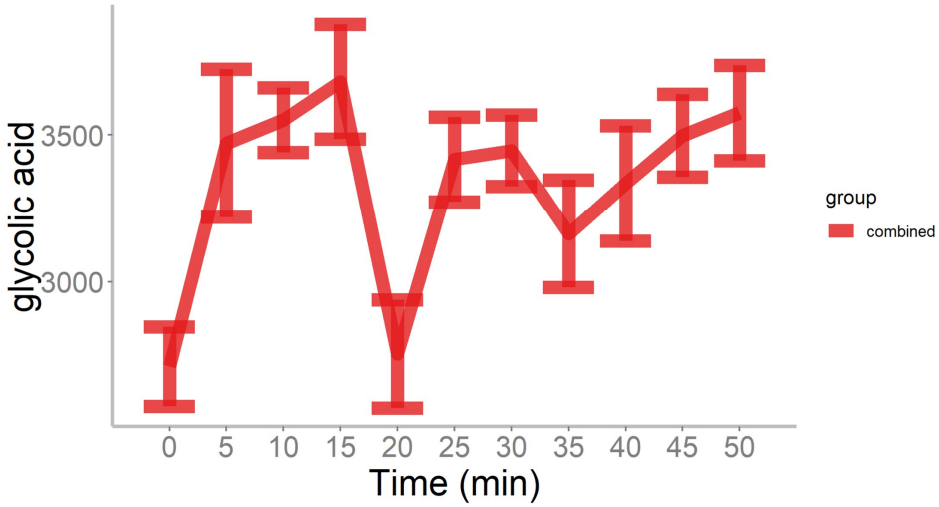

glyceric acid
2250
2000
1750
1500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

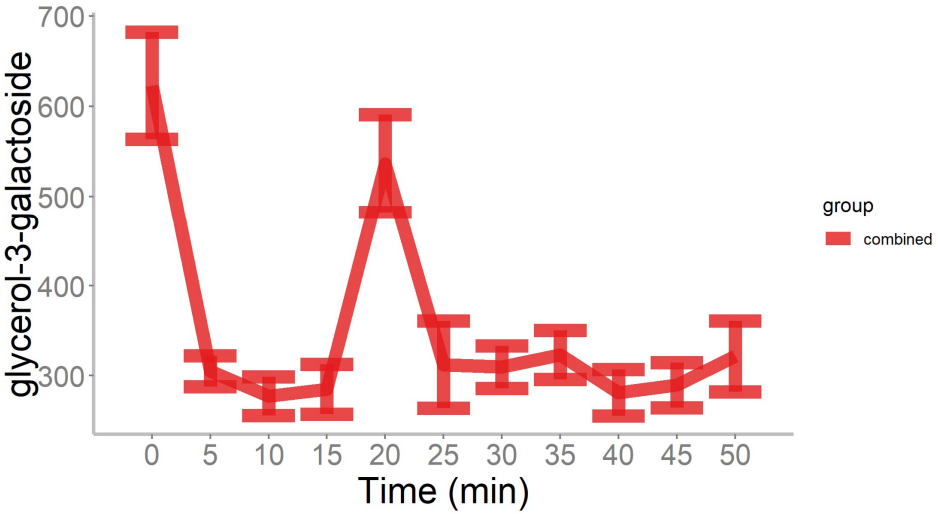

glycerol
110000
100000
90000
80000
70000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

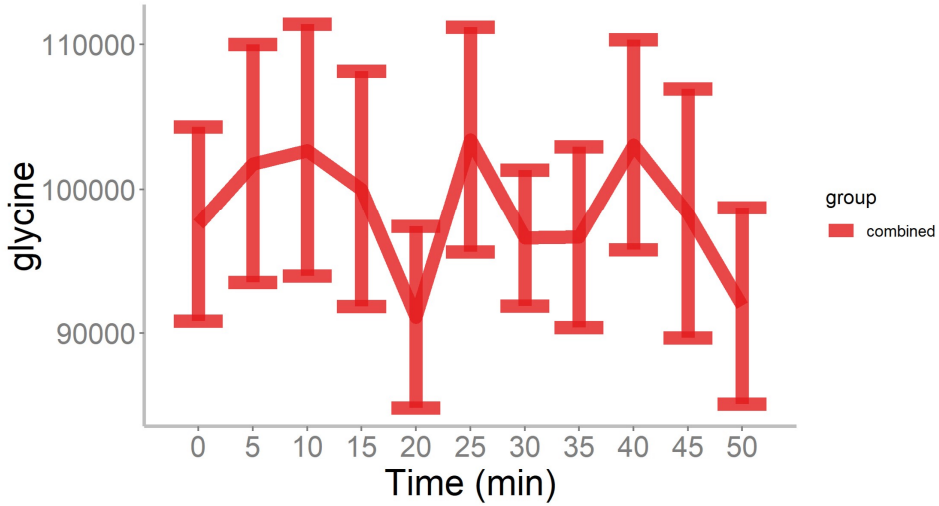

glutamylthreonine _by accurate r
700
650
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

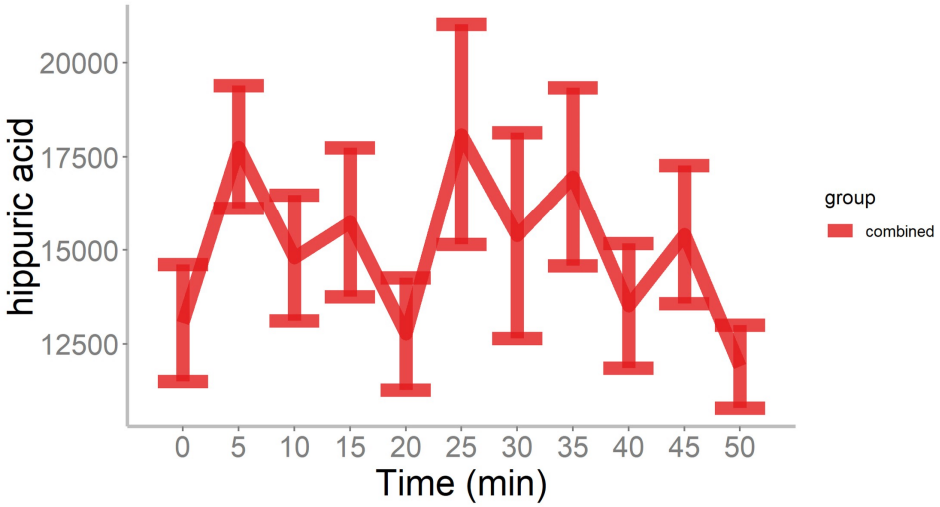

glycero-guloheptose NIST
450
400
350
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

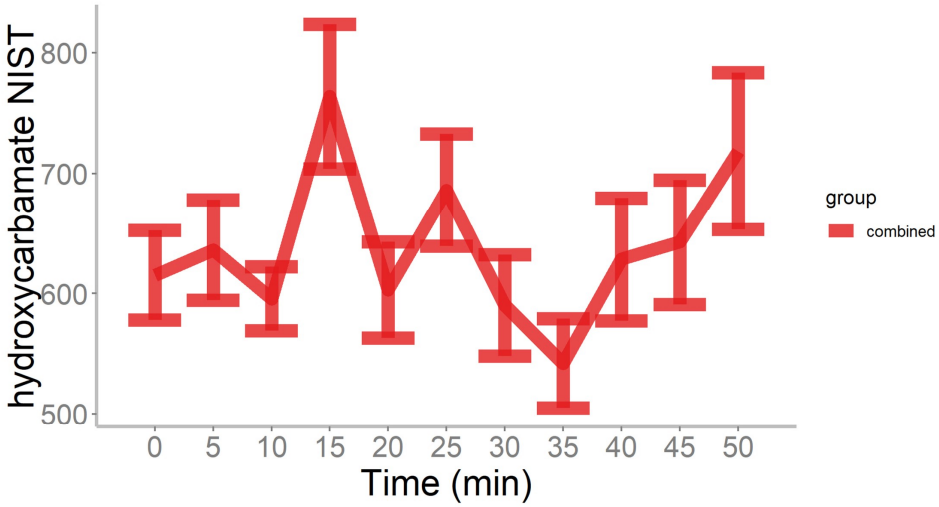

glycerol-alpha-phosphate
700
650
600
550
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

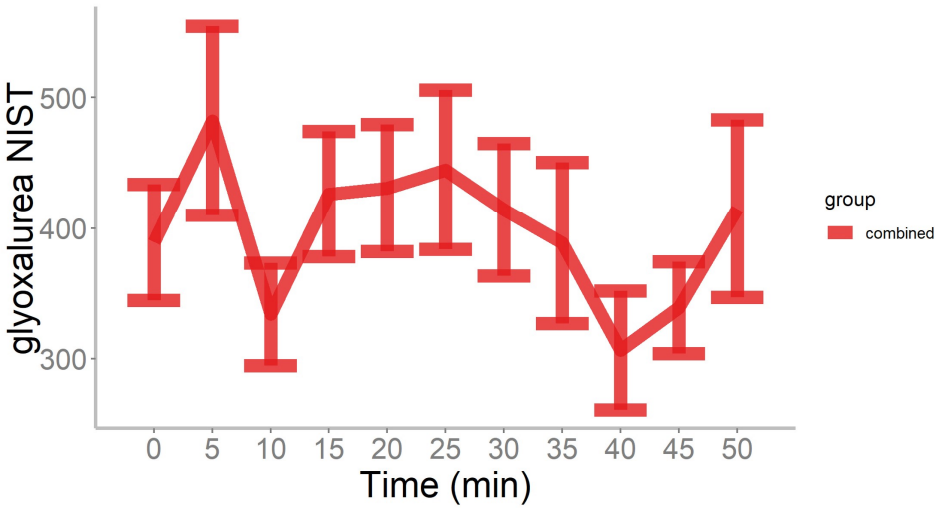

glycolic acid
3500
3000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

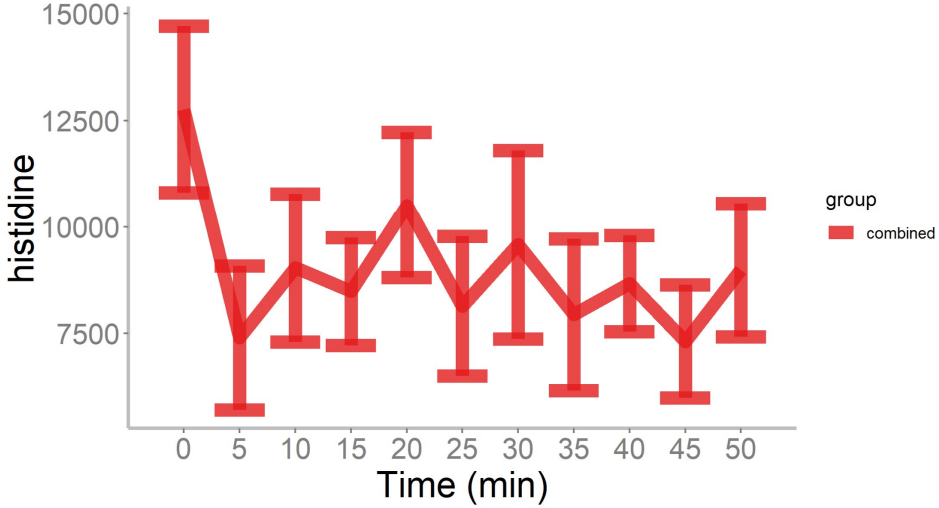

glycerol-3-galactoside
700
600
500
400
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

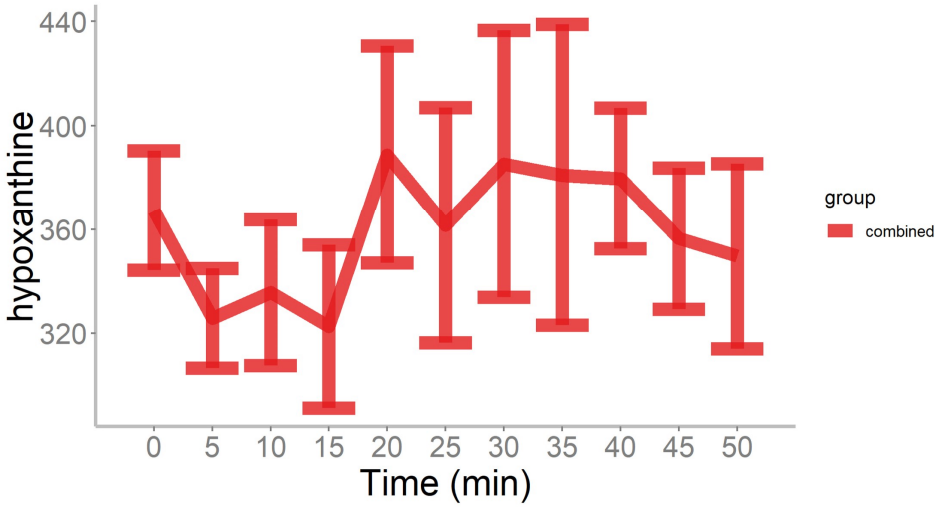

glycine
110000
100000
90000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

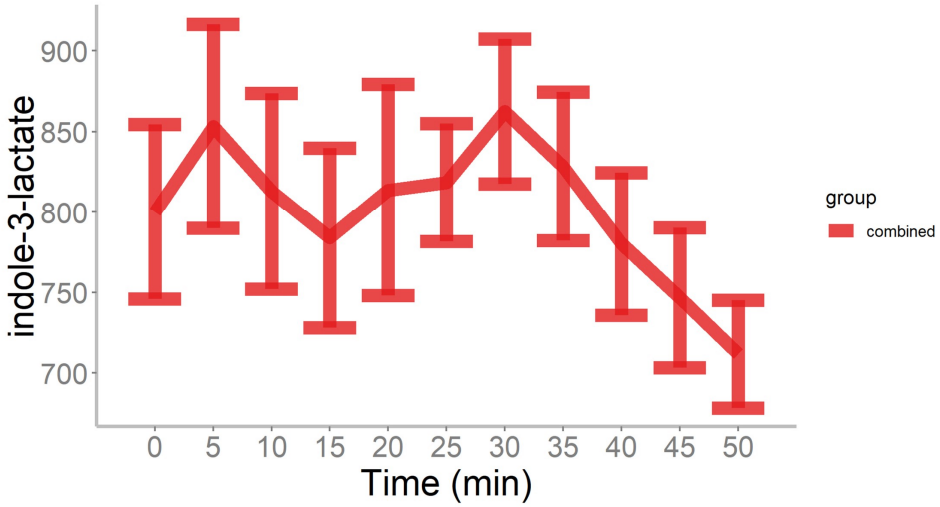

hippuric acid
20000
17500
15000
12500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

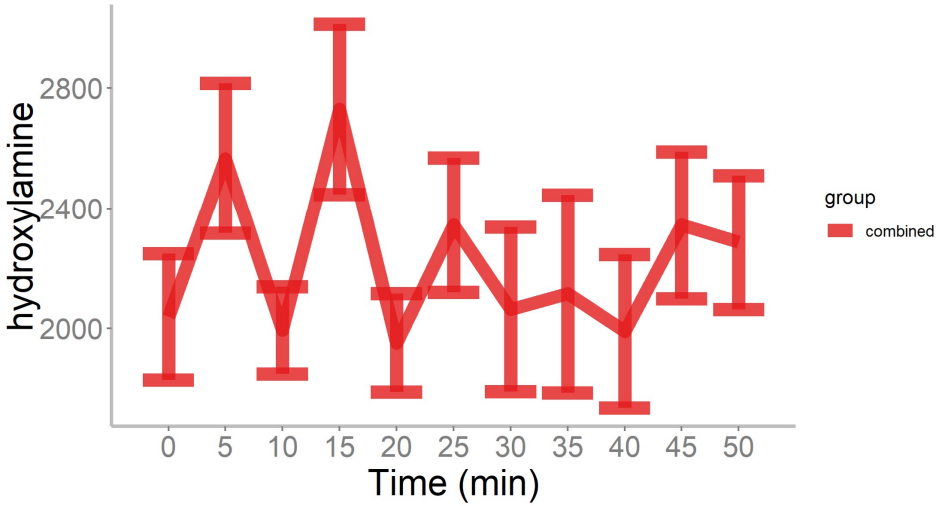

hydroxycarbamate NIST
800
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

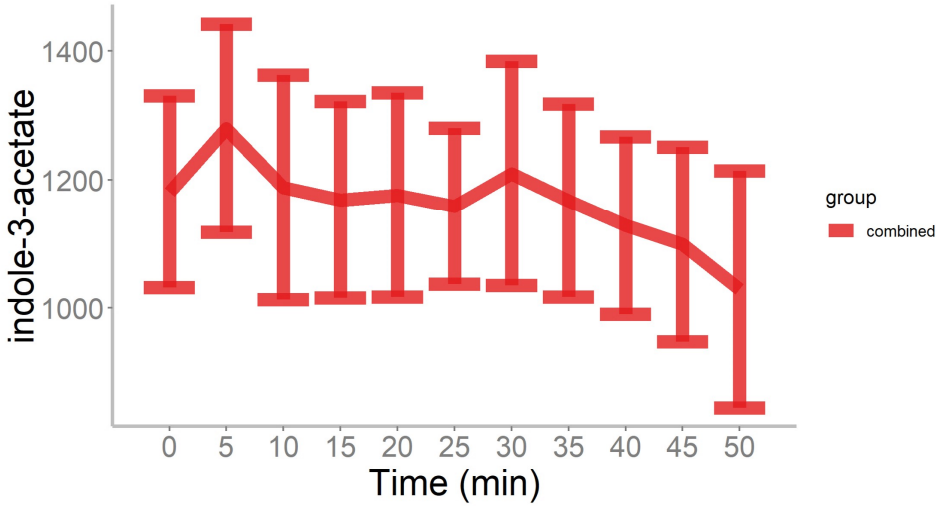

glyoxalurea NIST
500
400
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

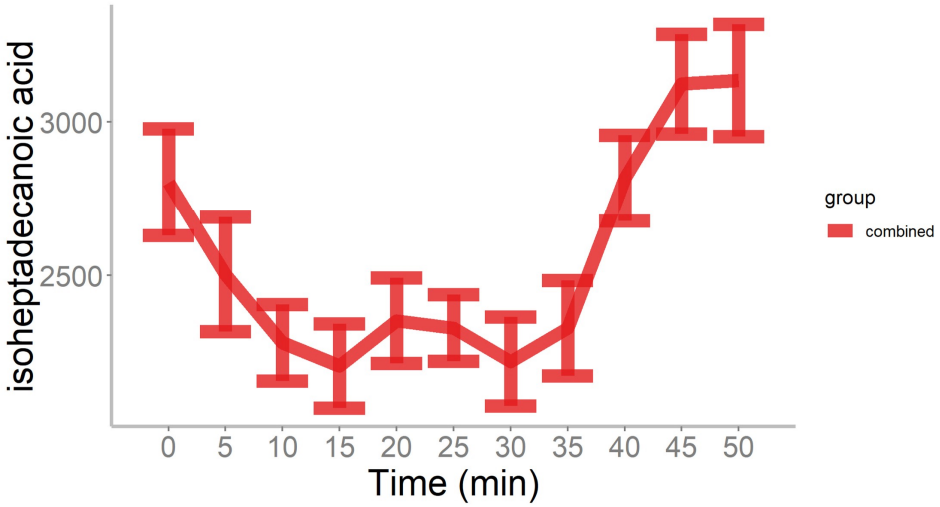

histidine
15000
12500
10000
7500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

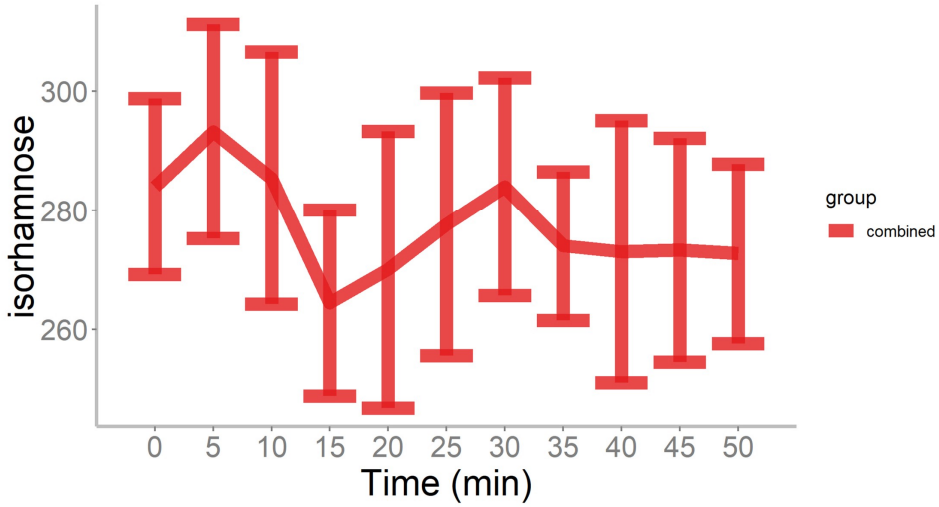

hypoxanthine
440
400
360
320
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

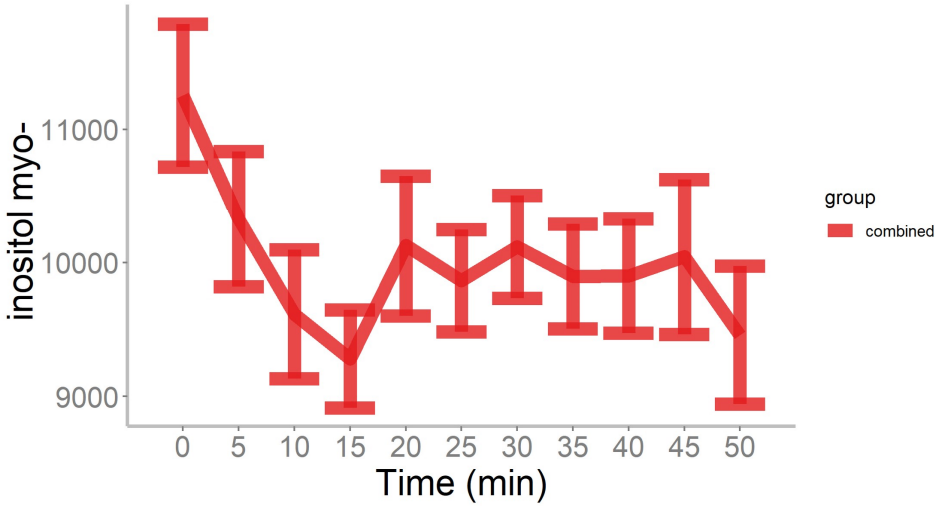

indole-3-lactate
900
850
800
750
700
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

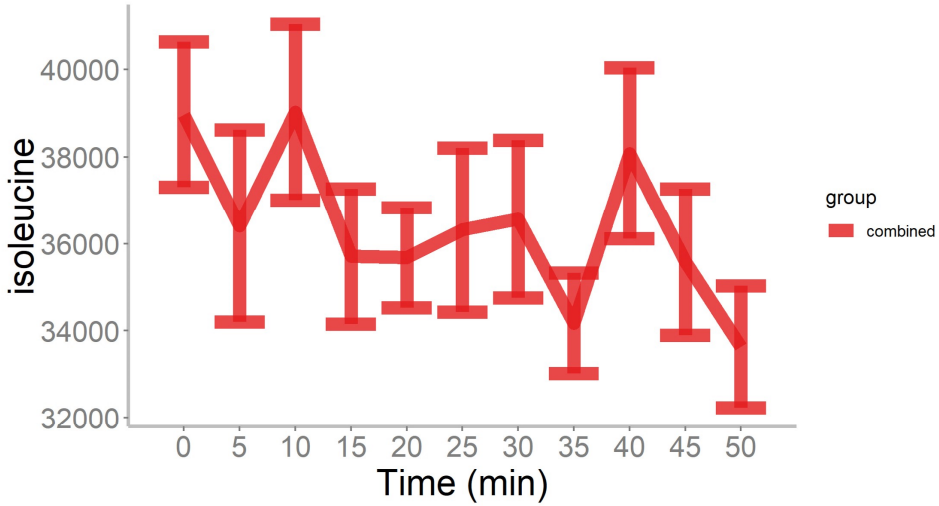

hydroxylamine
2800
2400
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

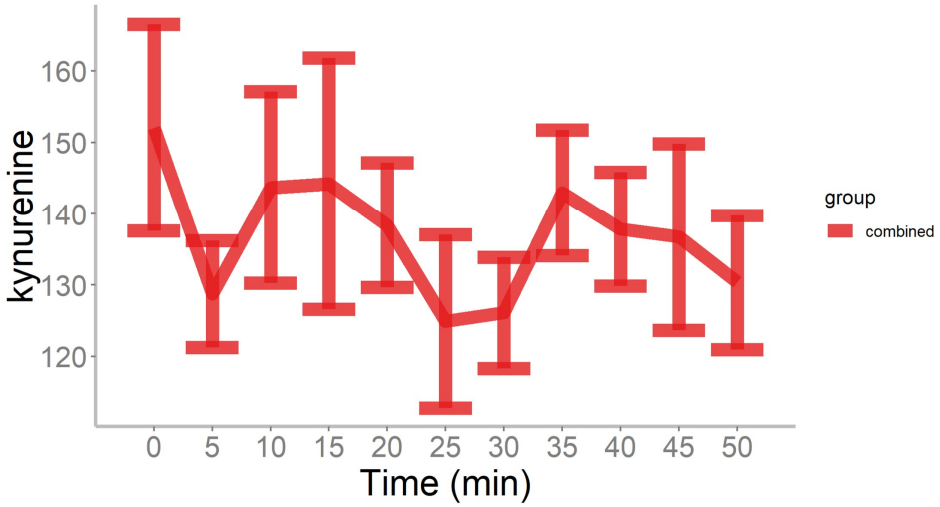

indole-3-acetate
1400
1200
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

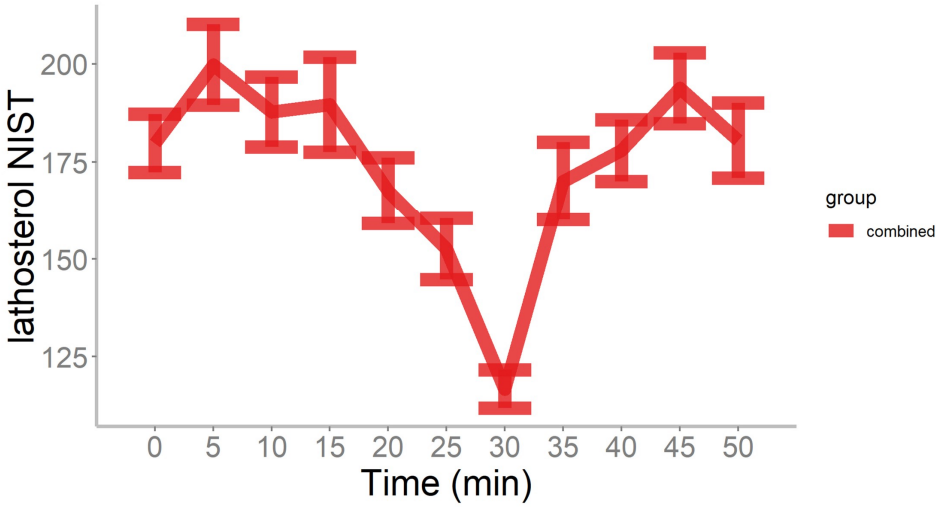

isoheptadecanoic acid
3000
2500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

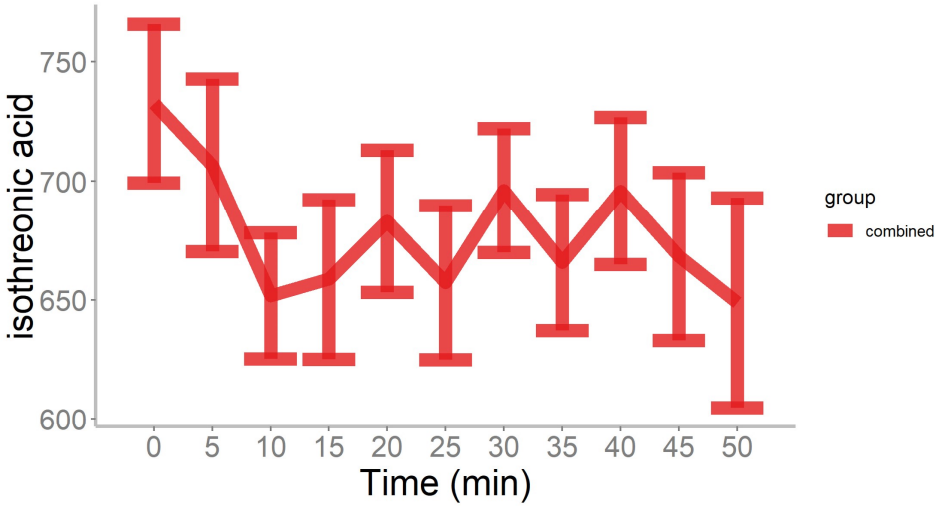

isorhamnose
300
280
260
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

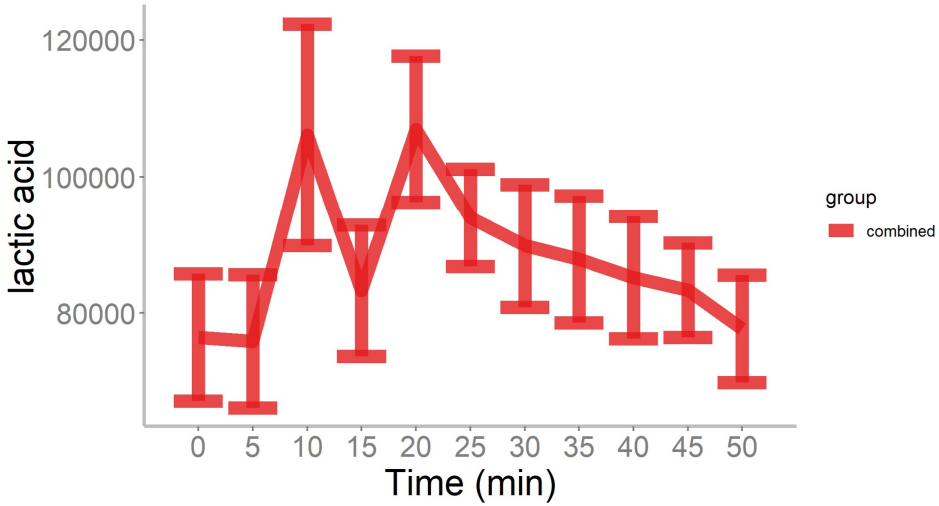

inositol myo-
11000
10000
9000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

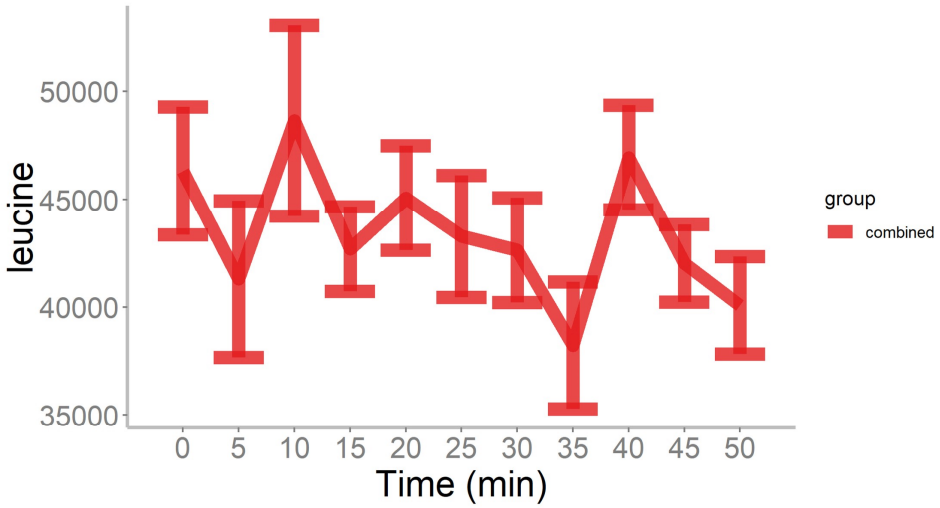

isoleucine
40000
38000
36000
34000
32000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

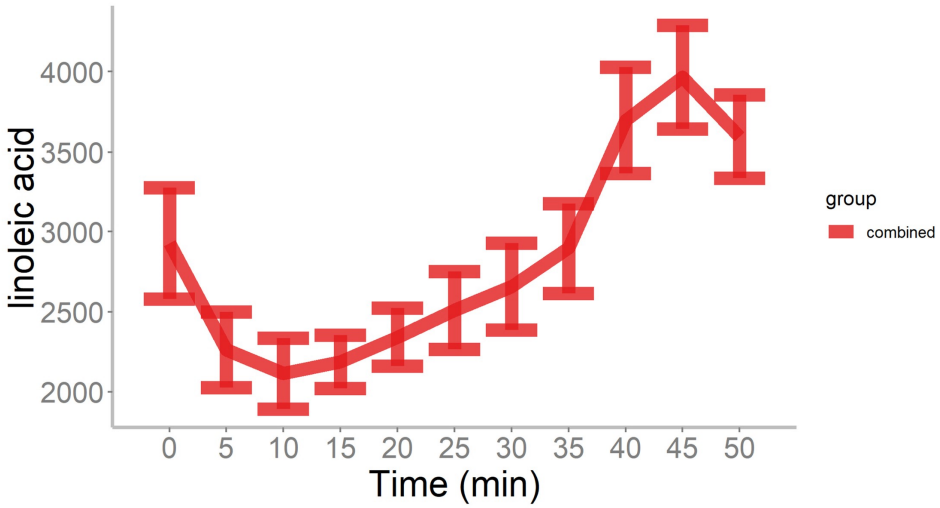

kynurenine
160
150
140
130
120
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


lathosterol NIST
200
175
150
125
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


isothreonic acid
750
700
650
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


lactic acid
120000
100000
80000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


leucine
50000
45000
40000
35000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


linoleic acid
4000
3500
3000
2500
2000
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Time (min)
group
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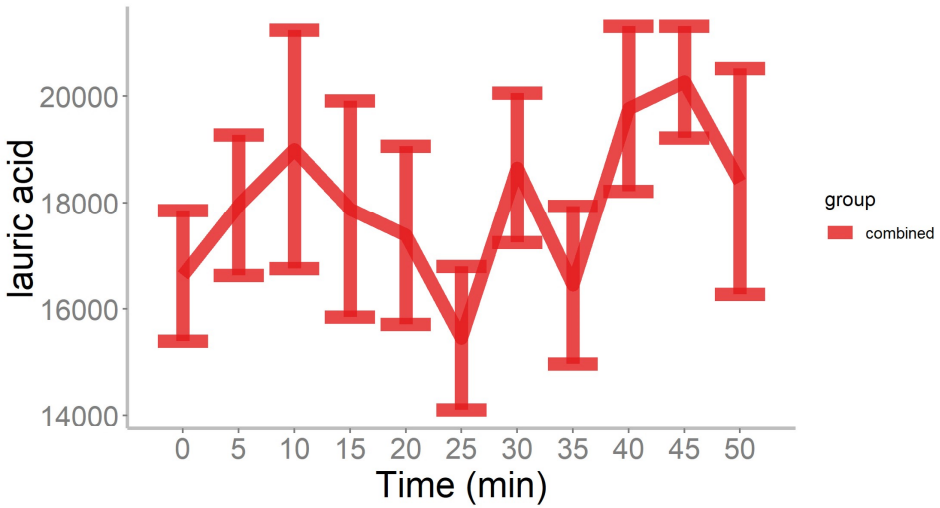
lauric acid
20000
18000
16000
14000
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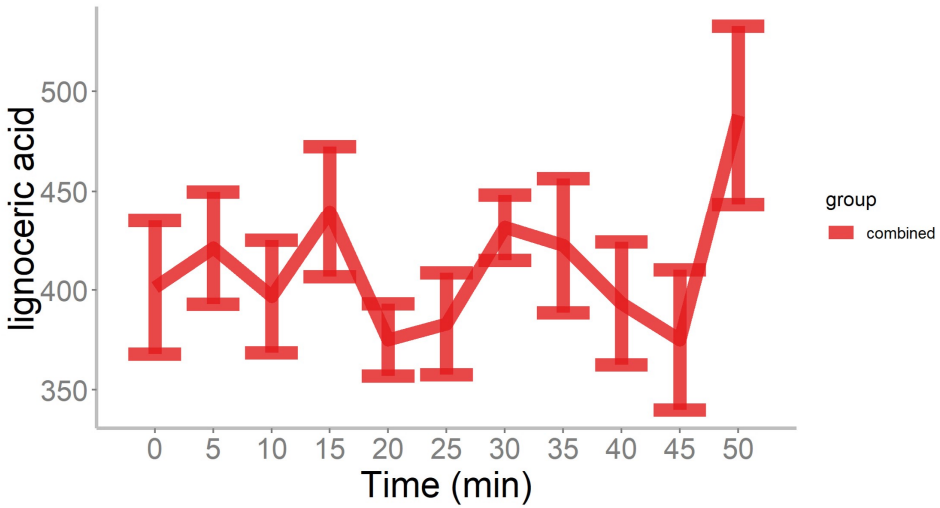
lignoceric acid
500
450
400
350
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Time (min)
group
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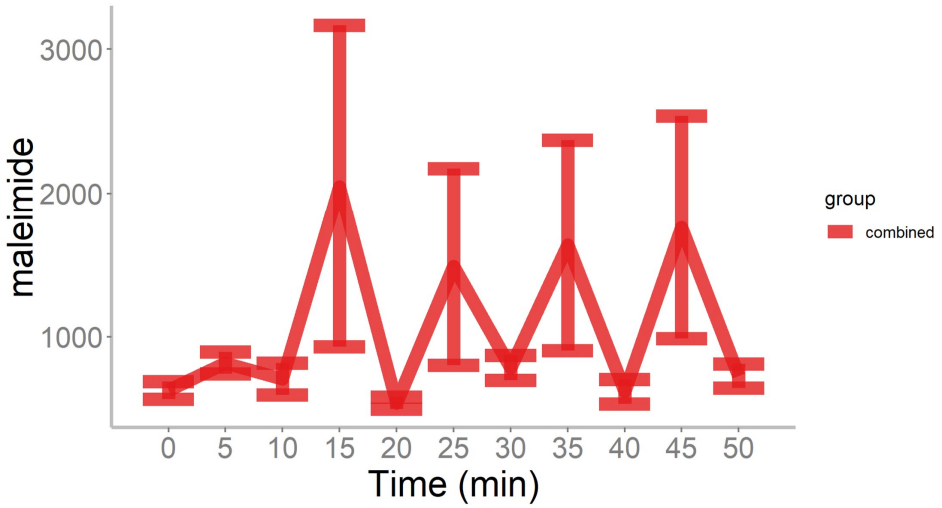
maleimide
3000
2000
1000
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Time (min)
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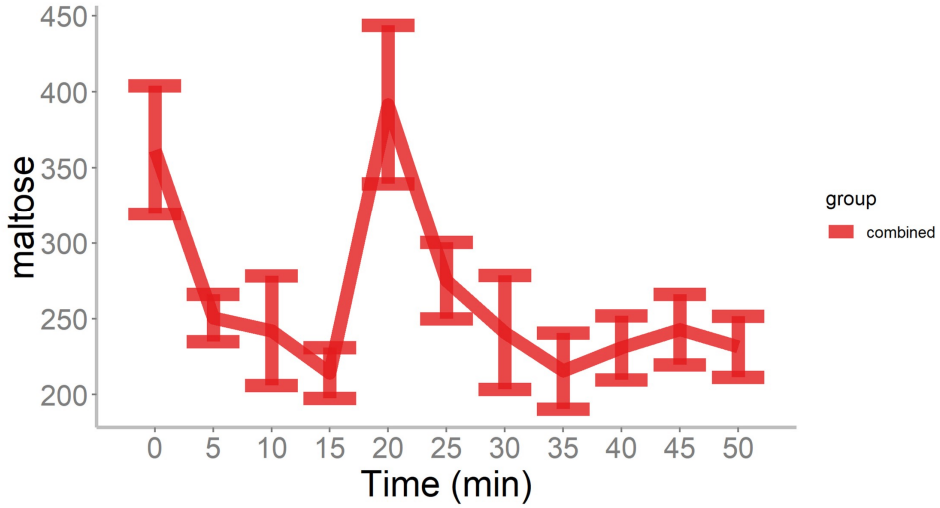
maltose
450
400
350
300
250
200
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Time (min)
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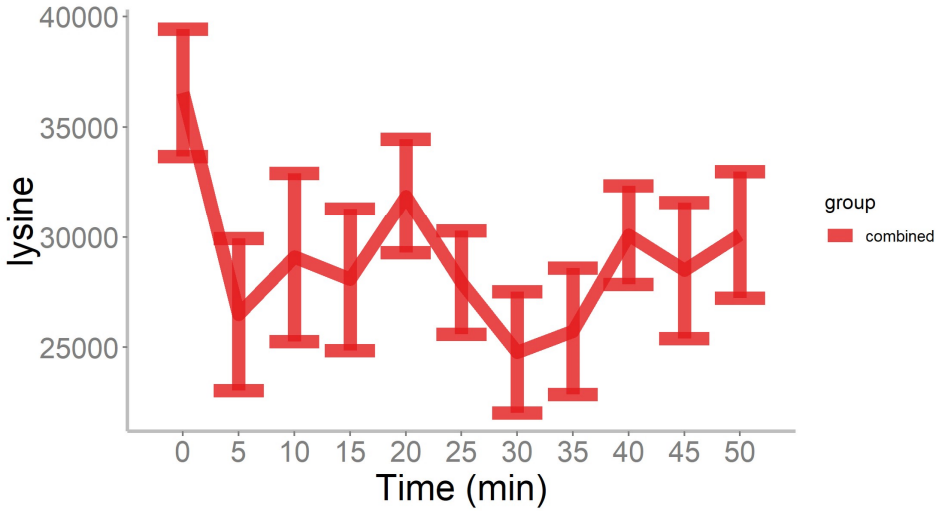
combined


lysine
40000
35000
30000
25000
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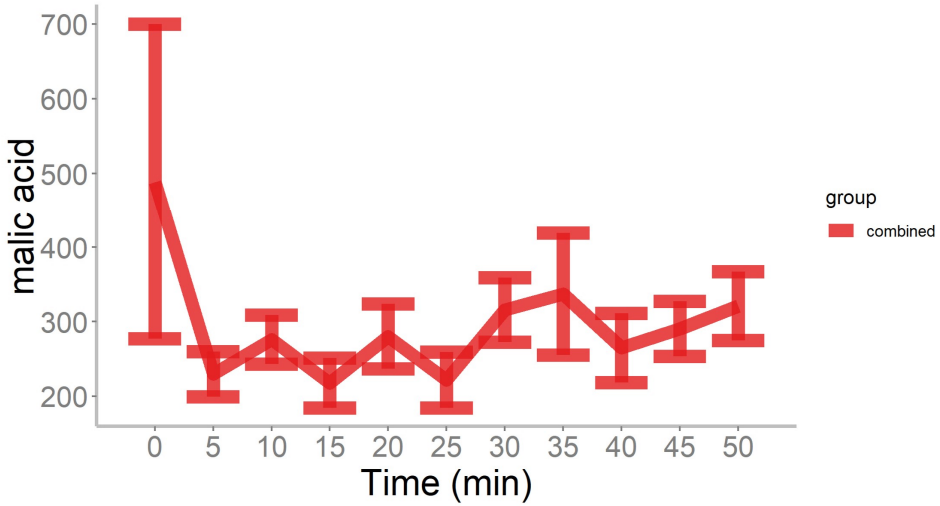
malic acid
700
600
500
400
300
200
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Time (min)
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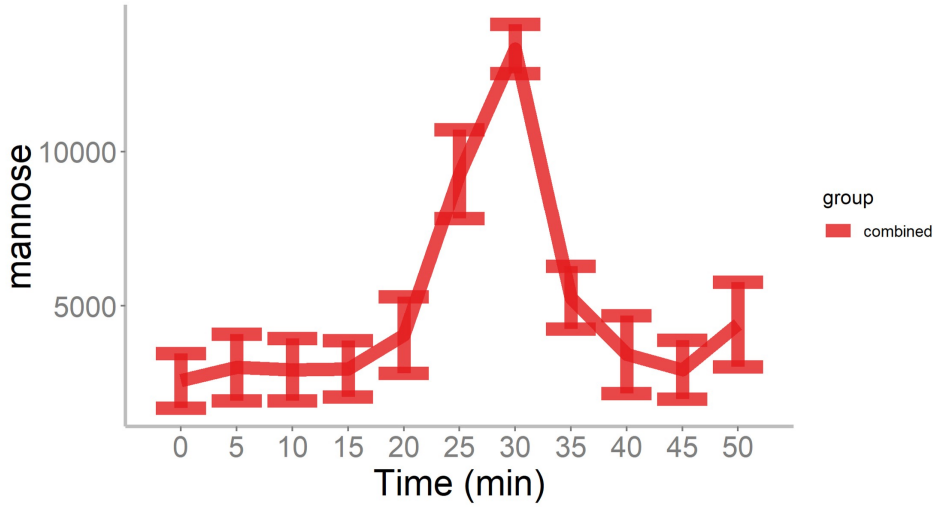
mannose
10000
5000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
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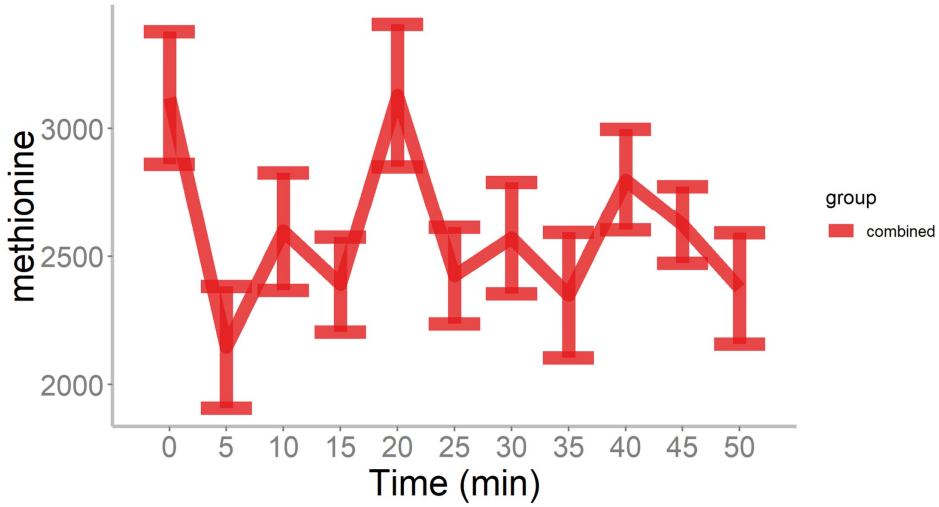
methionine
3000
2500
2000
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Time (min)
group
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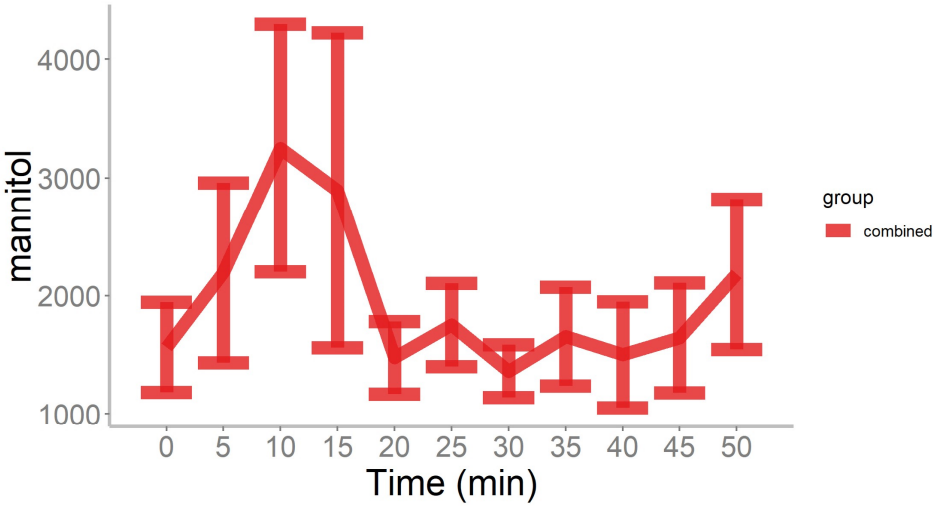
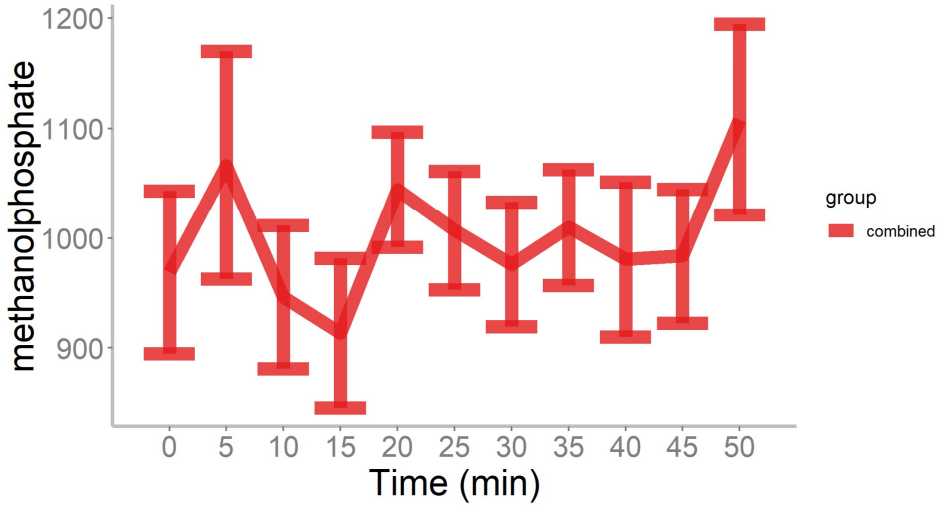
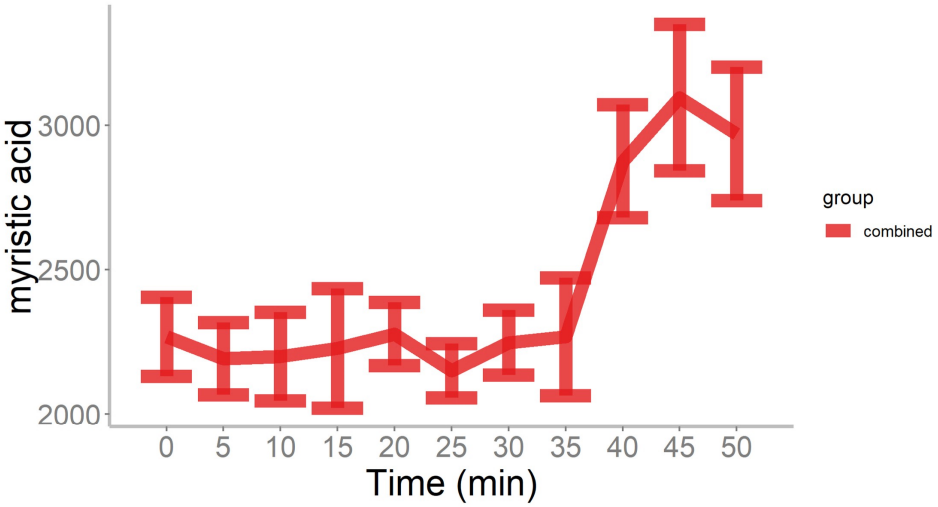
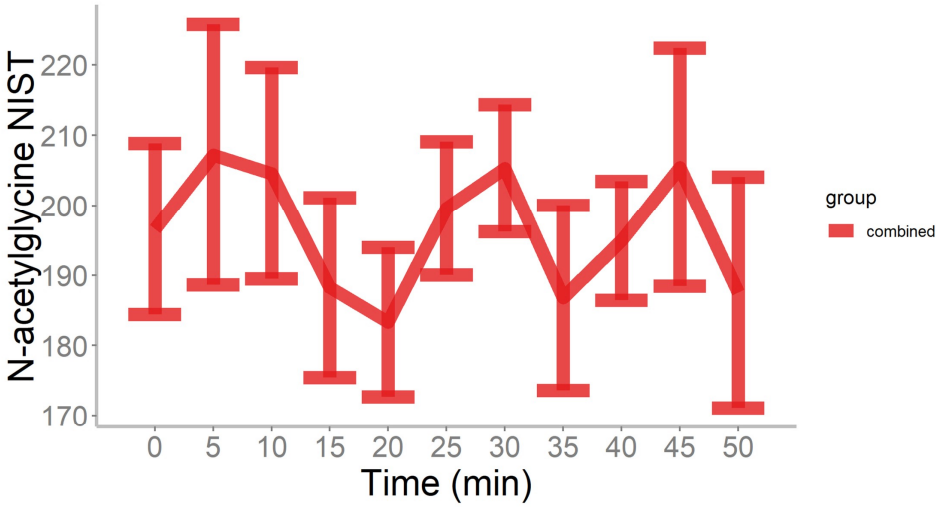
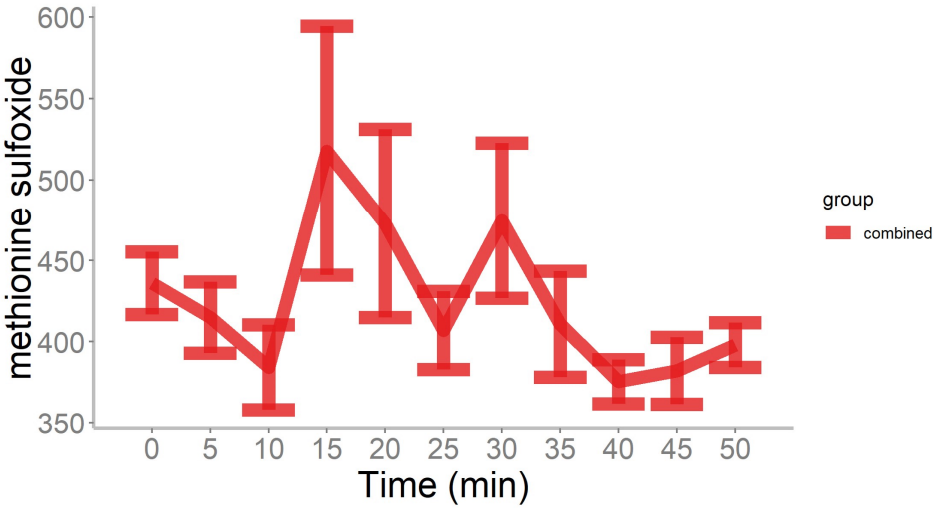
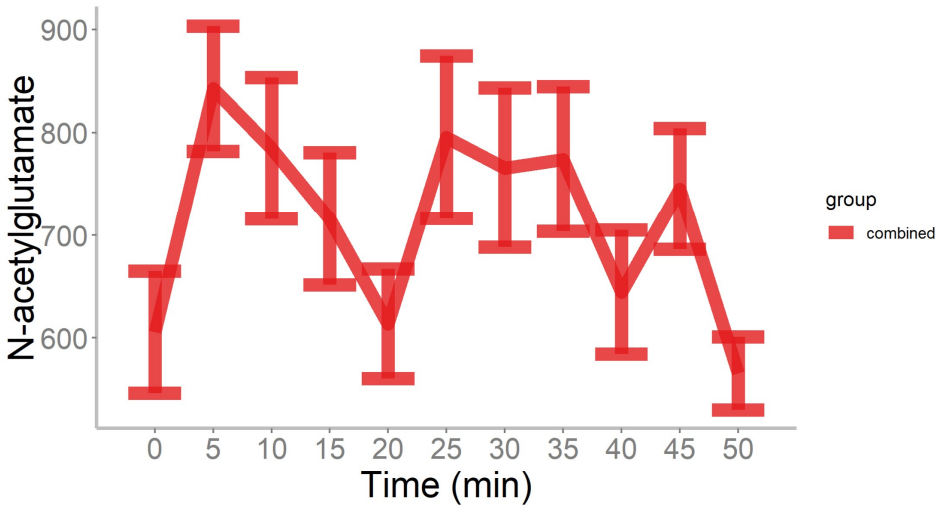

mannitol
4000
3000
2000
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

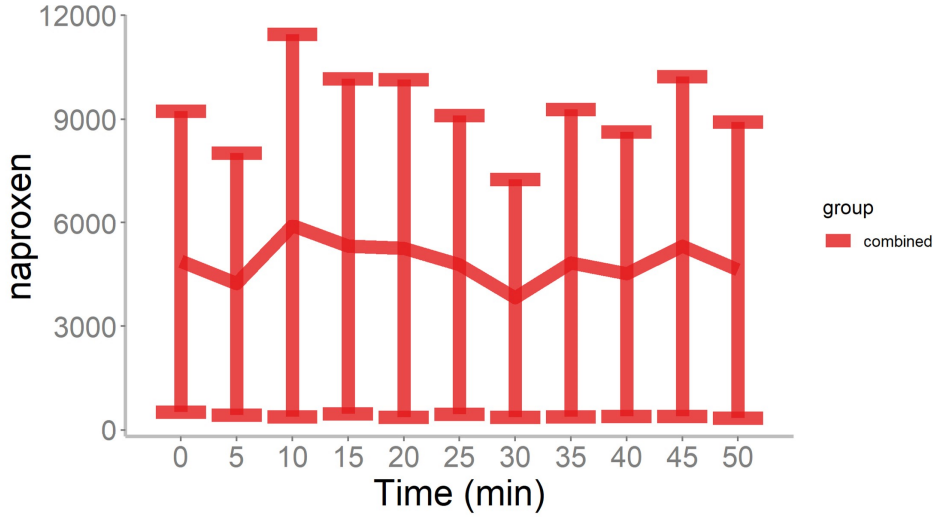

methanolphosphate
1200
1100
1000
900
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

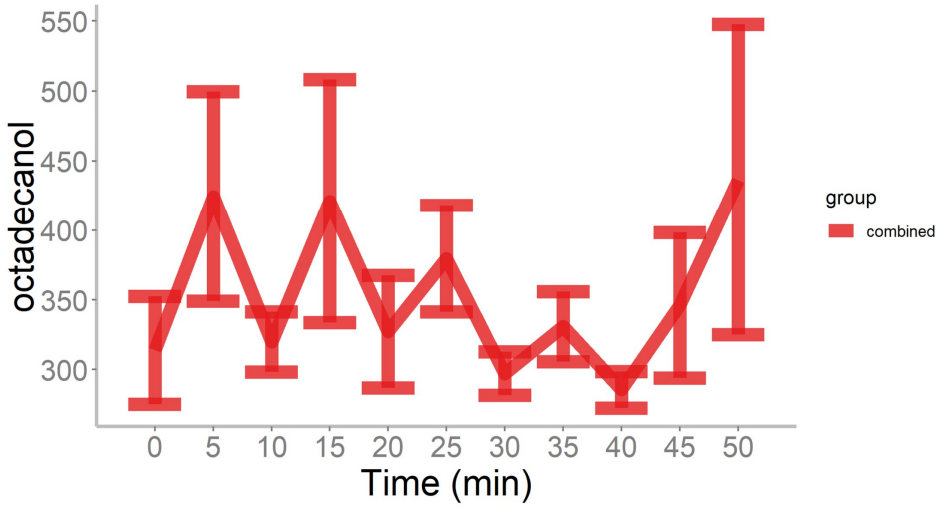

myristic acid
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

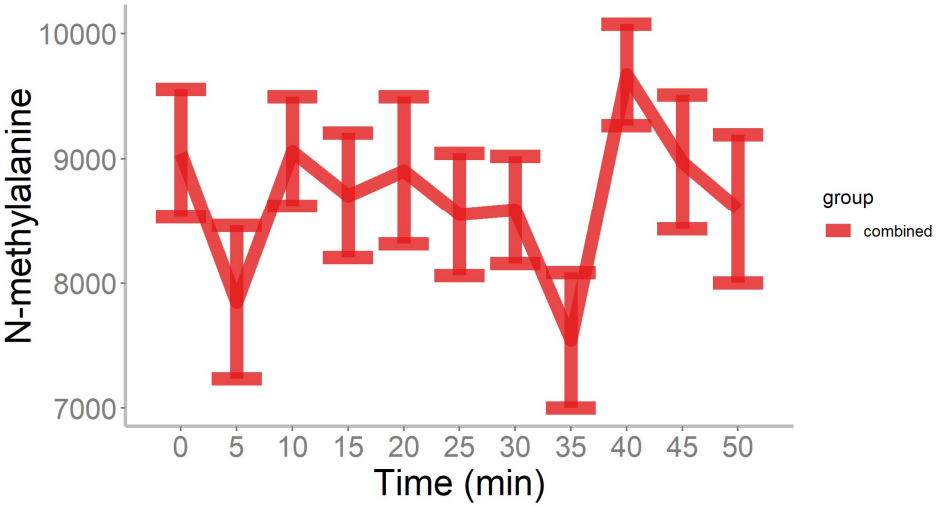

N-acetylglycine NIST
220
210
200
190
180
170
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

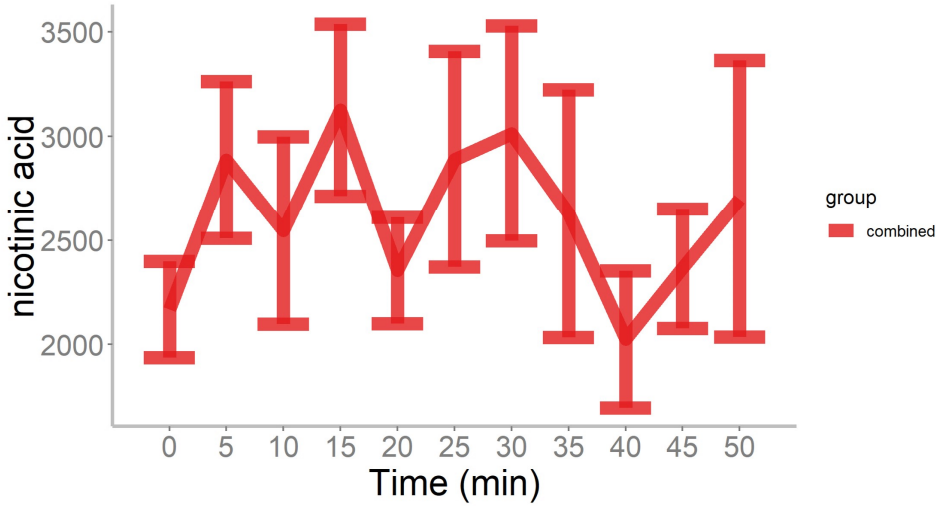

methionine sulfoxide
600
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

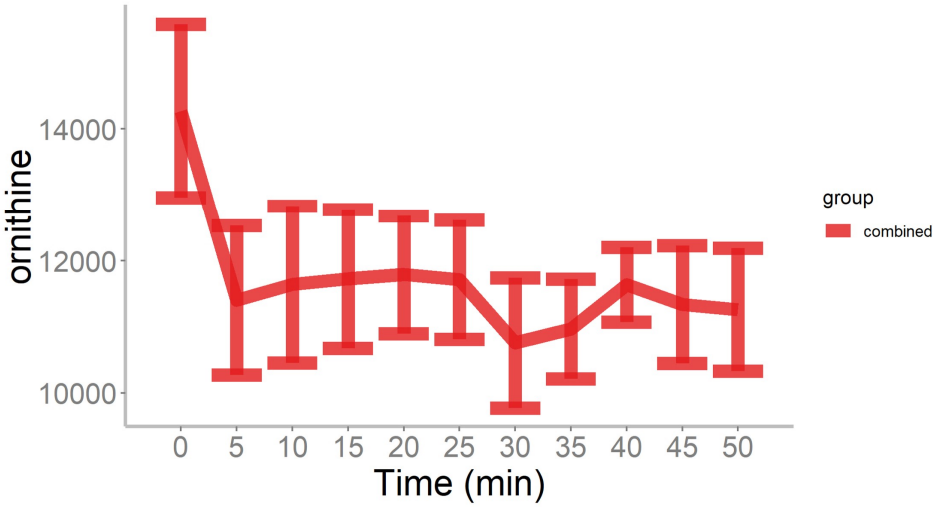

N-acetylglutamate
900
800
700
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

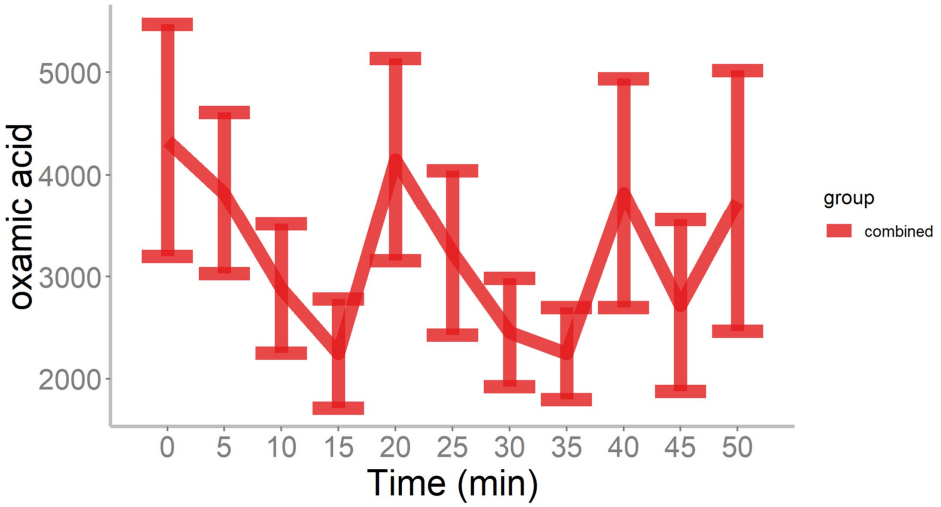

naproxen
12000
9000
6000
3000
0
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

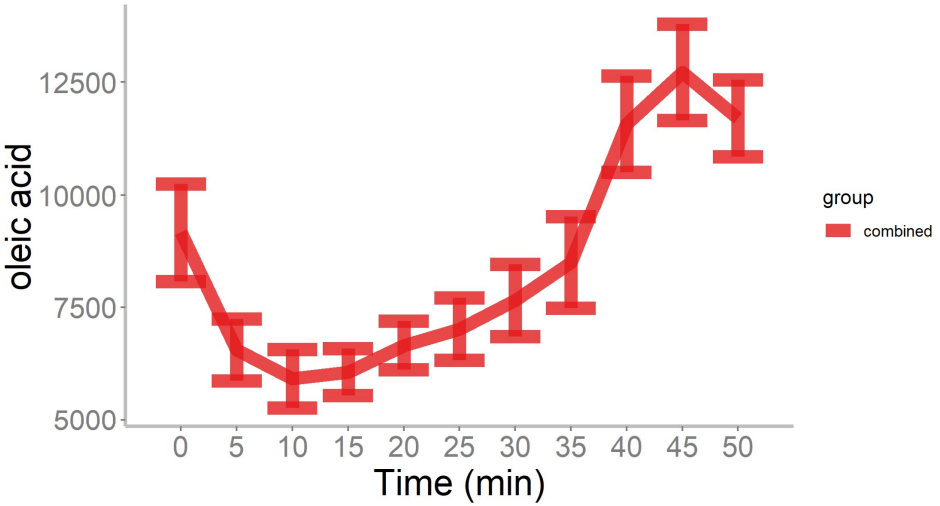

octadecanol
550
500
450
400
350
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

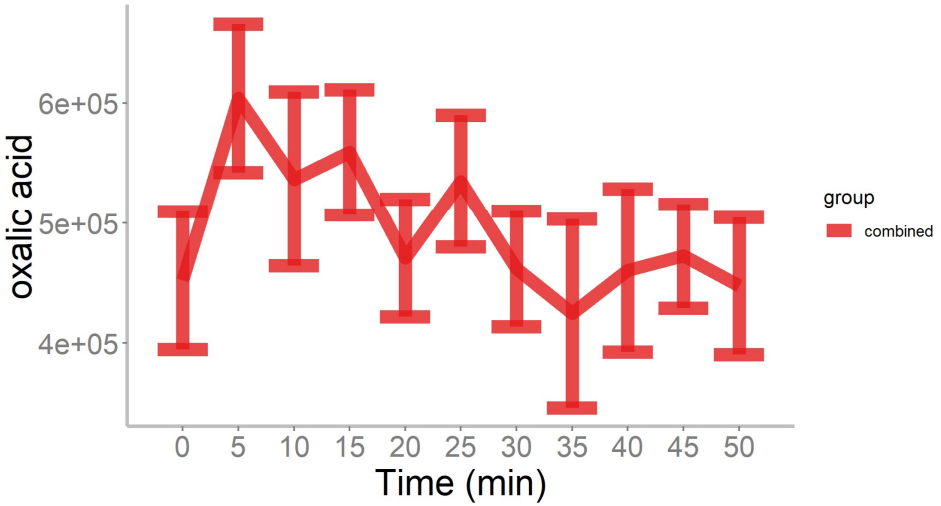

N-methylalanine
10000
9000
8000
7000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

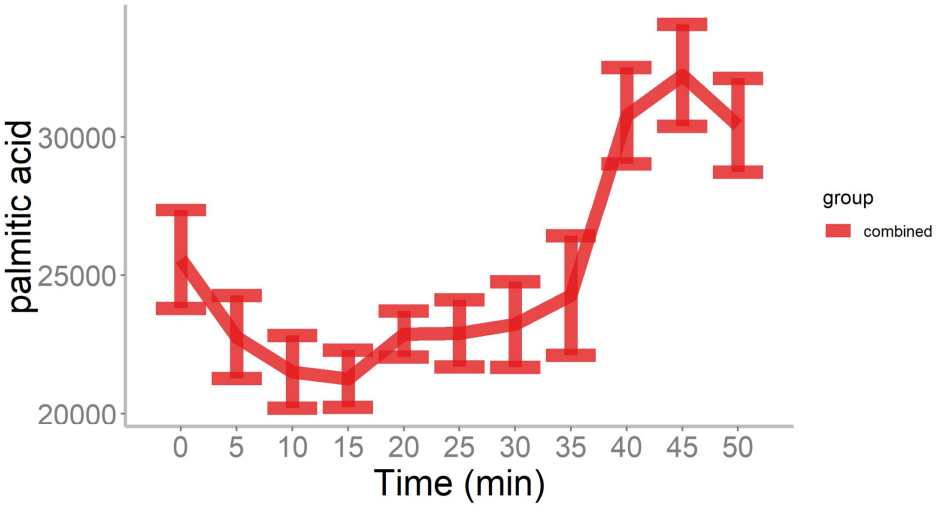

nicotinic acid
3500
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

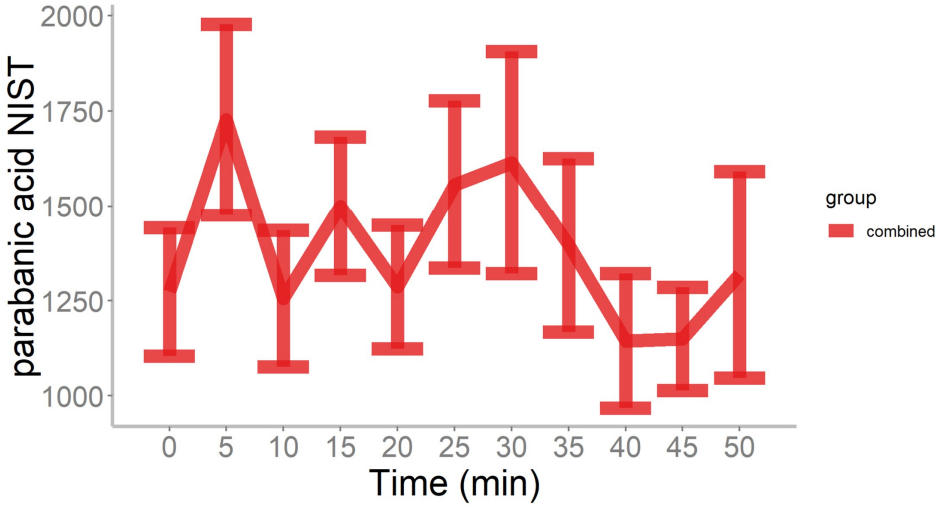

ornithine
14000
12000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

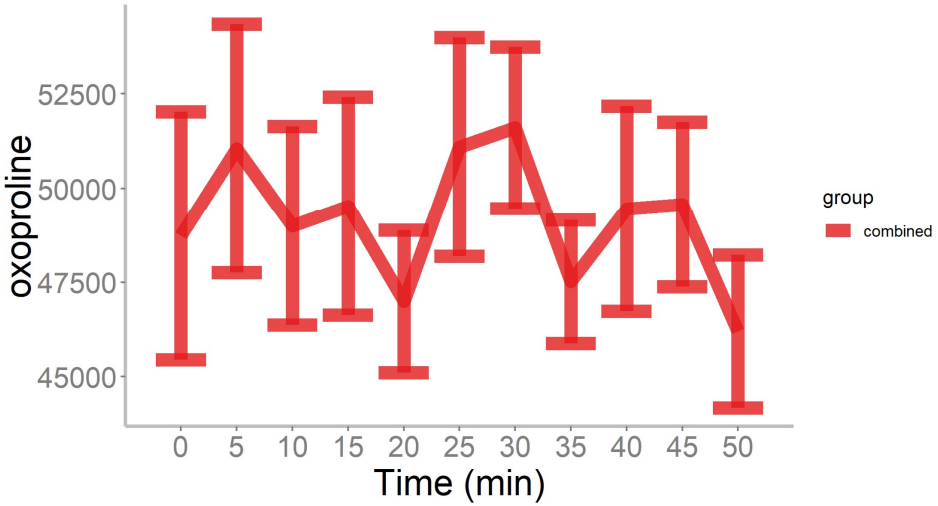

oxamic acid
5000
4000
3000
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

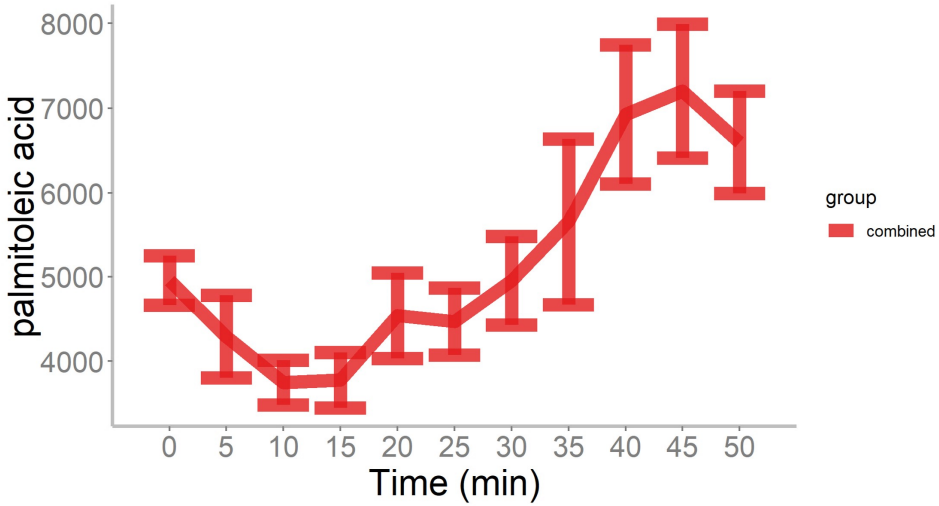

oleic acid
12500
10000
7500
5000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

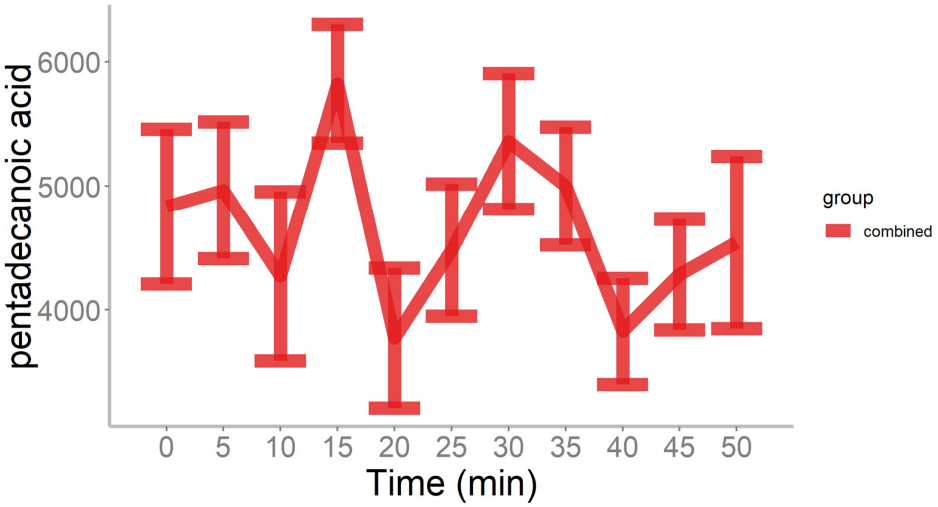

oxalic acid
6e+05
5e+05
4e+05
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

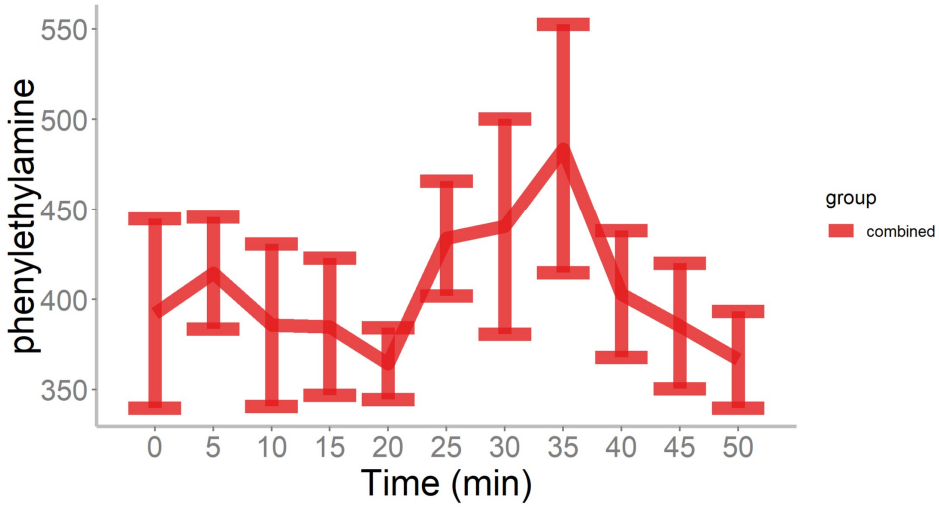

palmitic acid
30000
25000
20000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

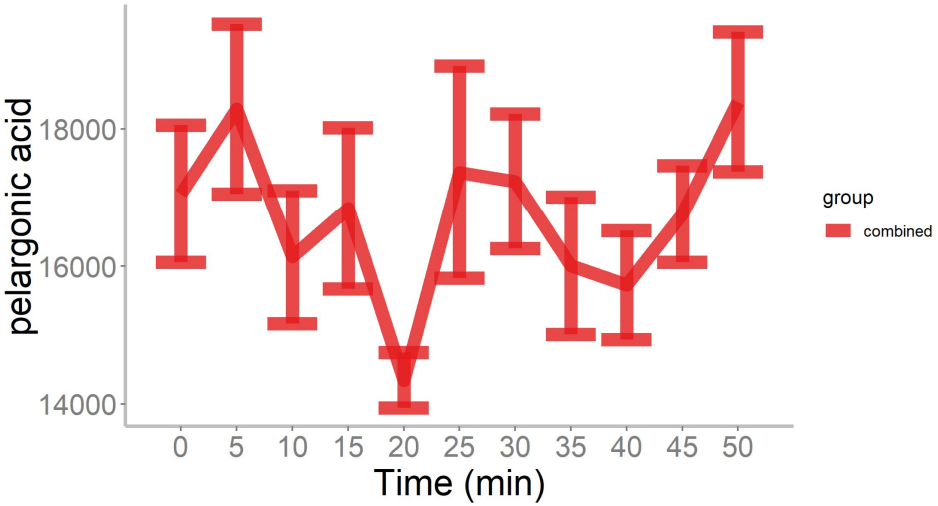

parabanic acid NIST
2000
1750
1500
1250
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

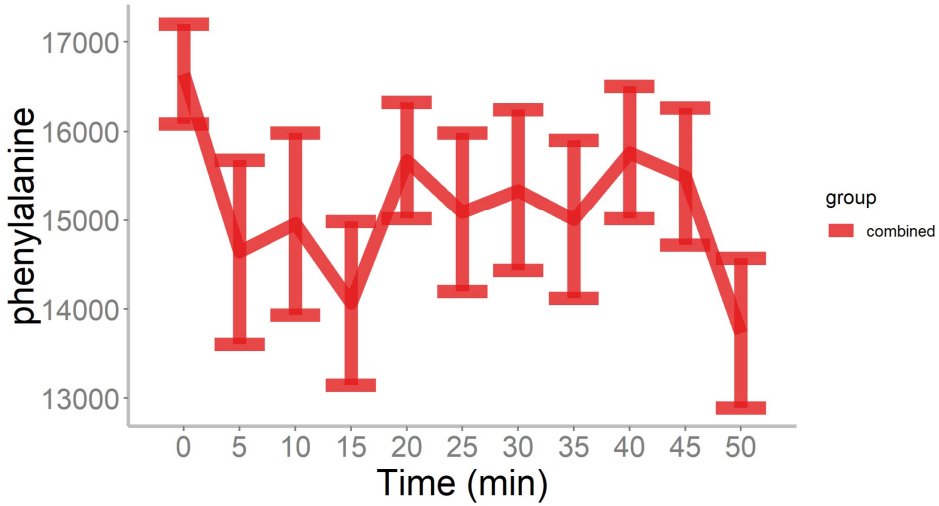

oxoproline
52500
50000
47500
45000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

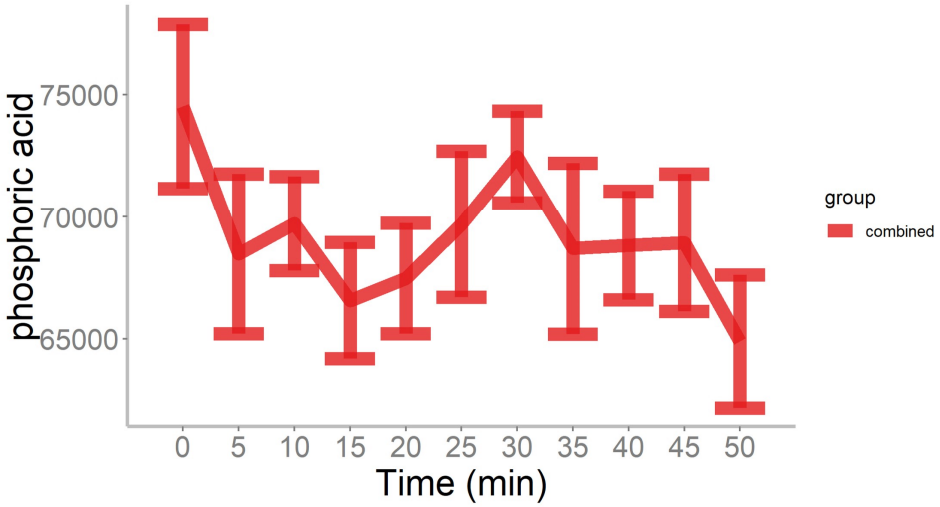

palmitoleic acid
8000
7000
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

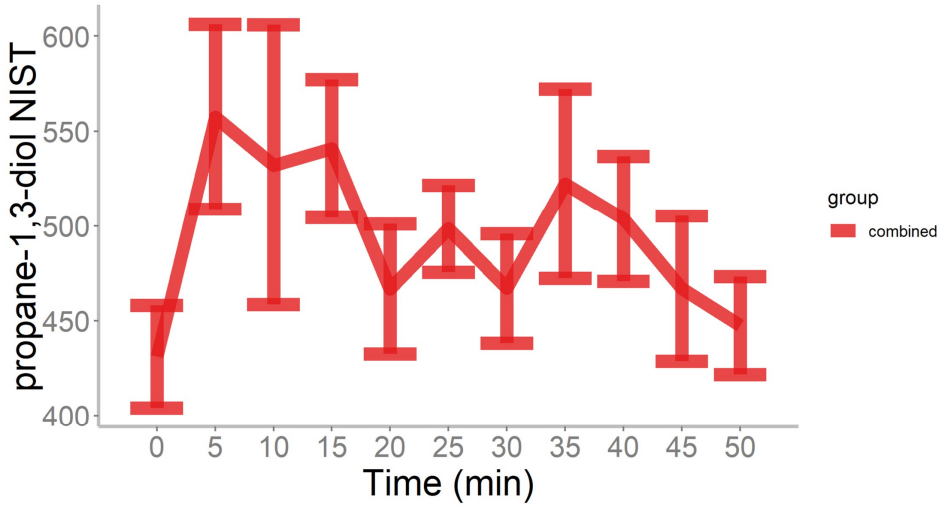

pentadecanoic acid
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

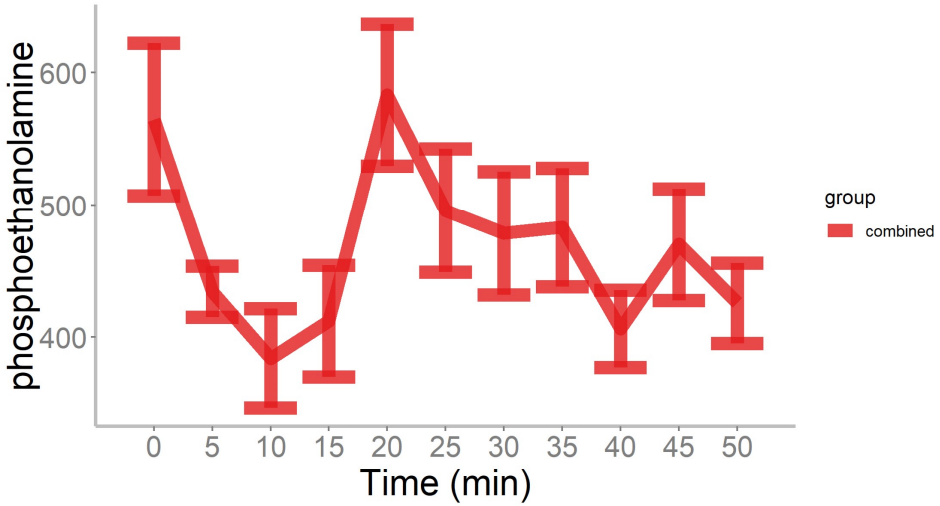

phenylethylamine
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

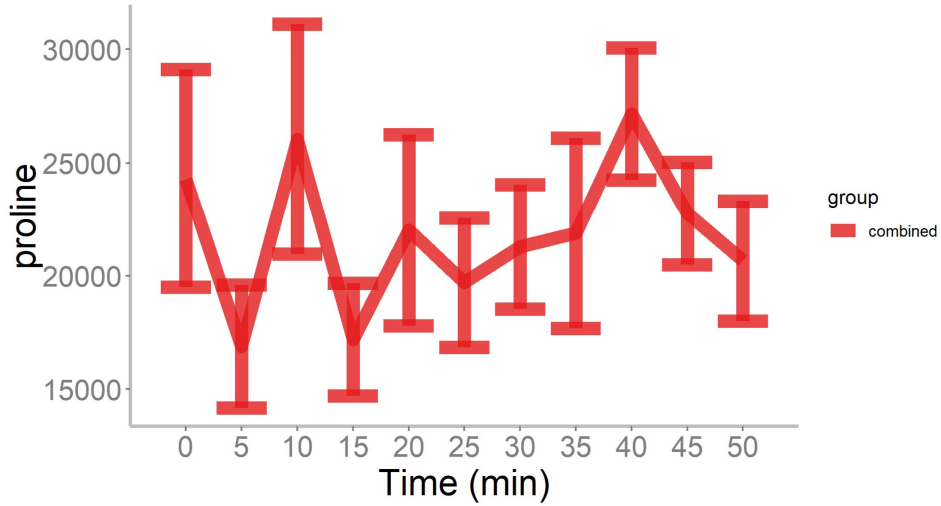

pelargonic acid
18000
16000
14000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

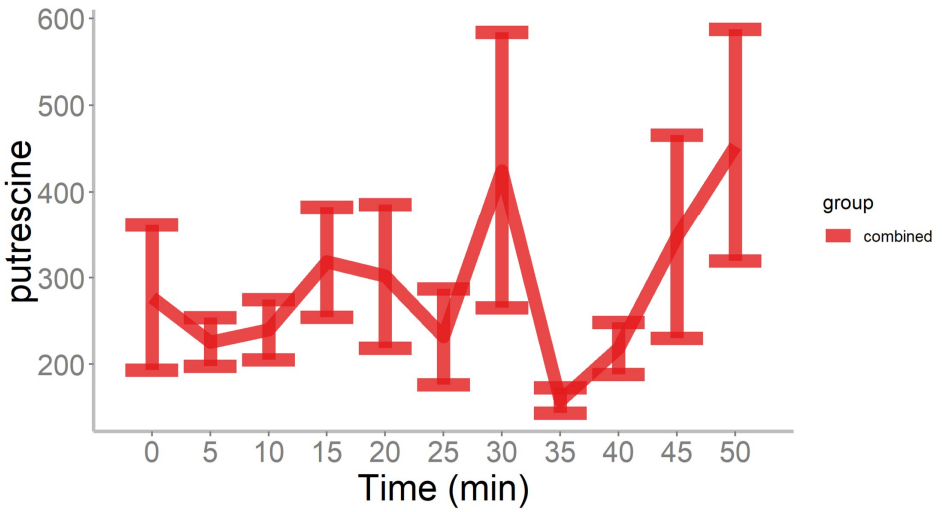

phenylalanine
17000
16000
15000
14000
13000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

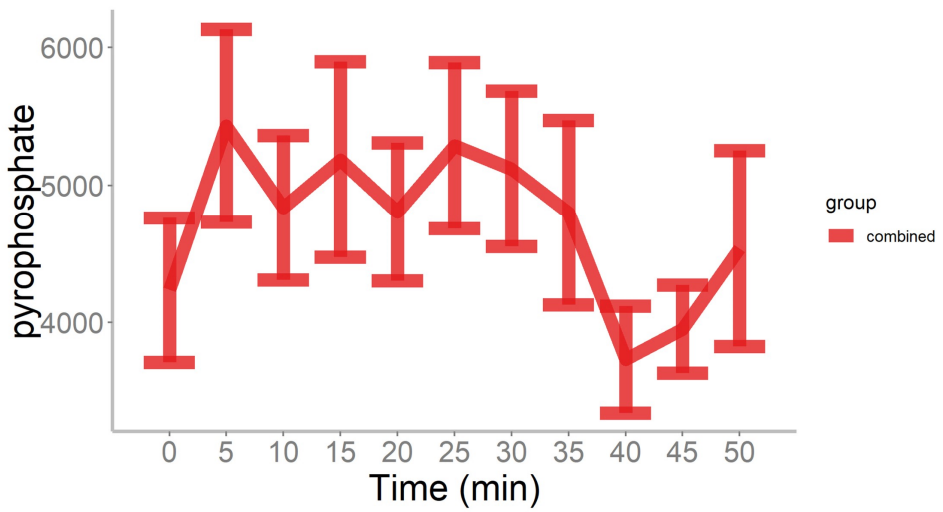

phosphoric acid
75000
70000
65000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

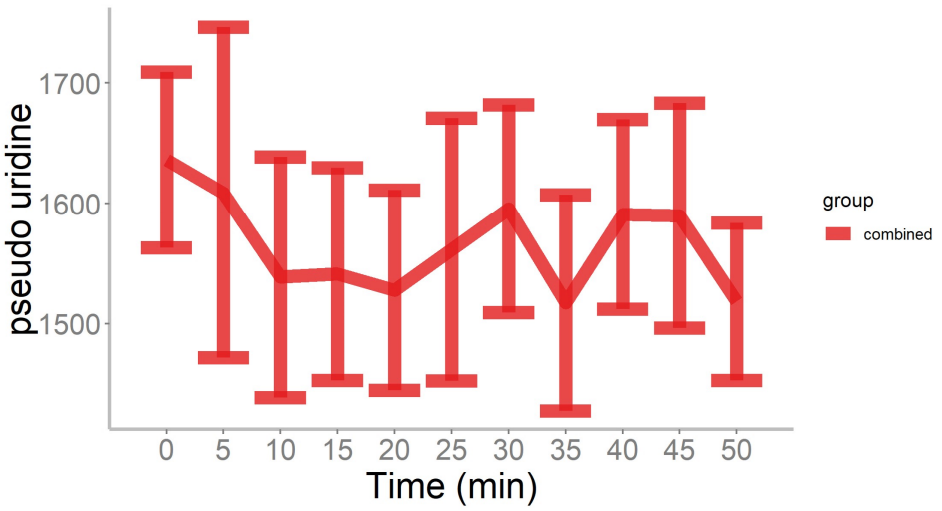

propane-1,3-diol NIST
600
550
500
450
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

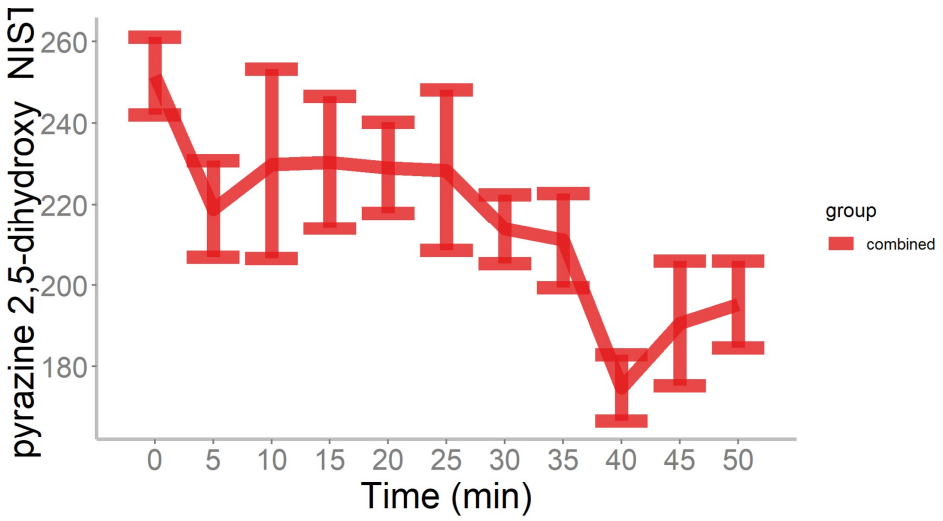

phosphoethanolamine
600
500
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

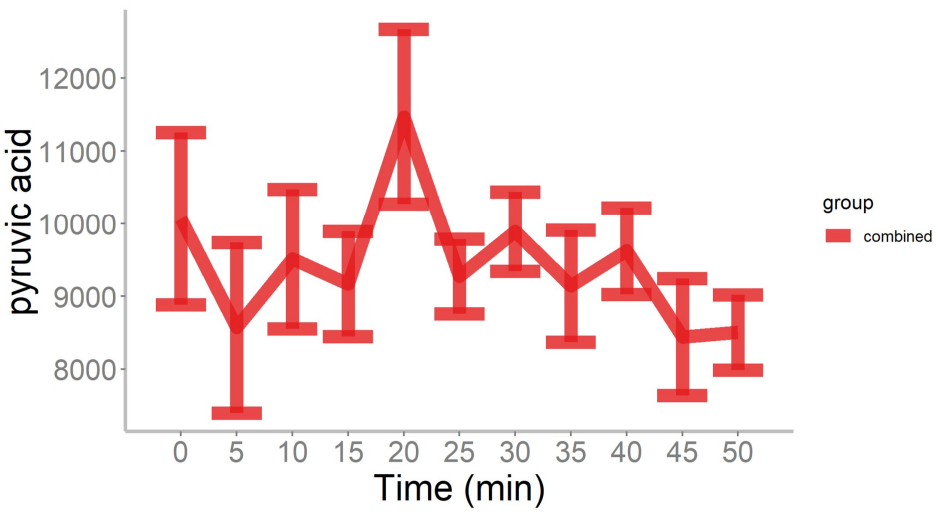

proline
30000
25000
20000
15000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

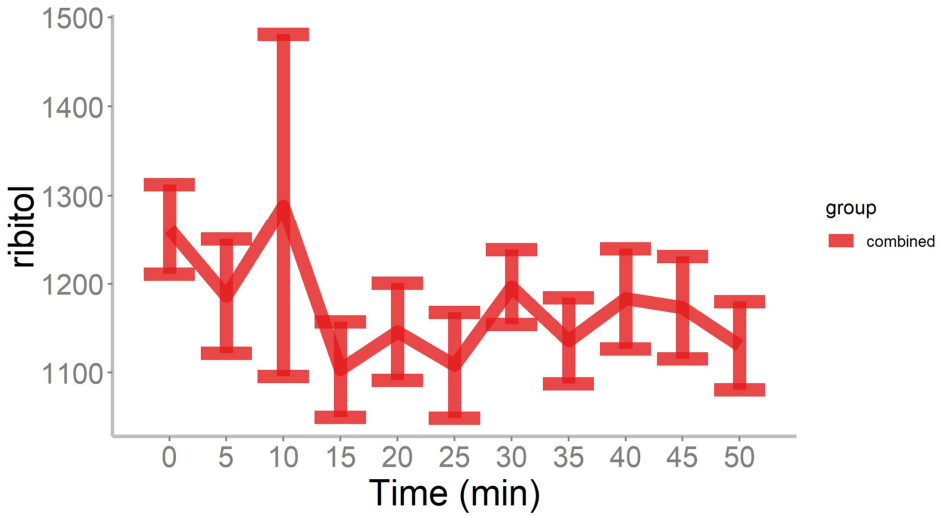

putrescine
600
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

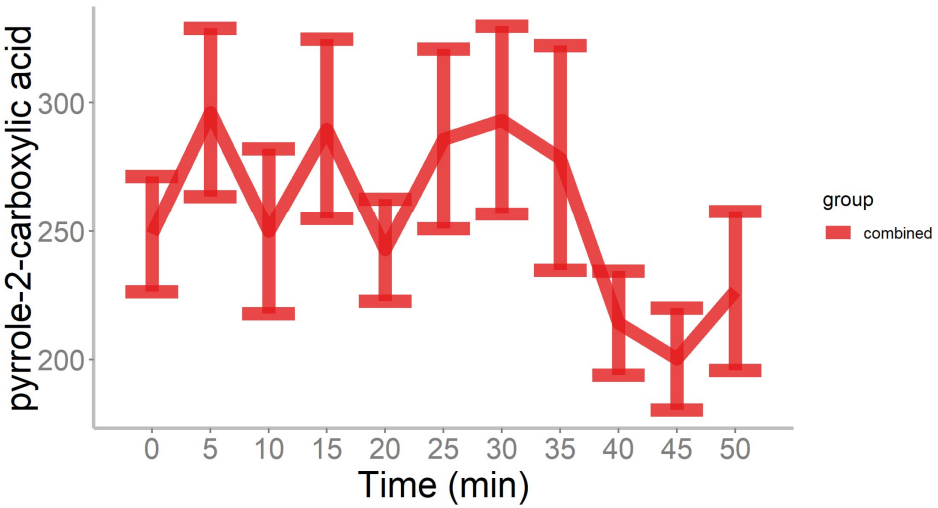

pyrophosphate
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

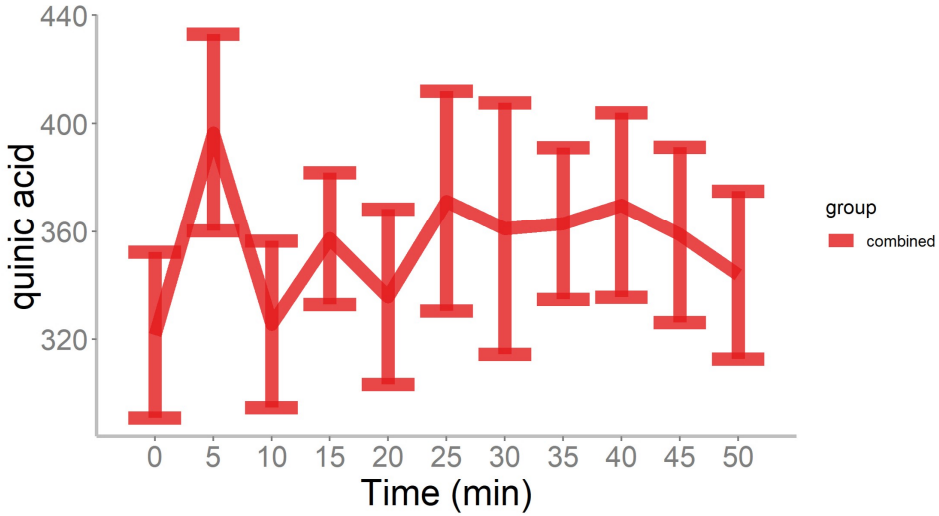

pseudo uridine
1700
1600
1500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

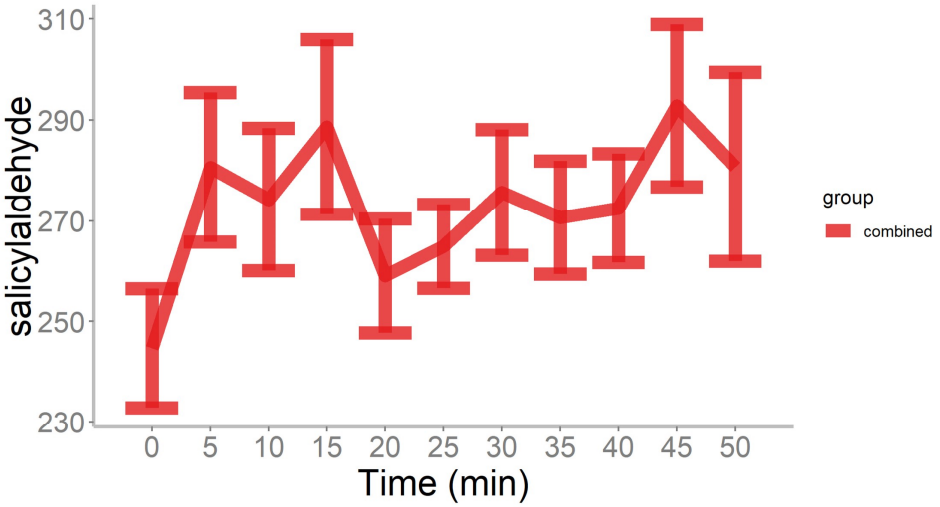

pyrazine 2,5-dihydroxy NIST
260
240
220
200
180
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

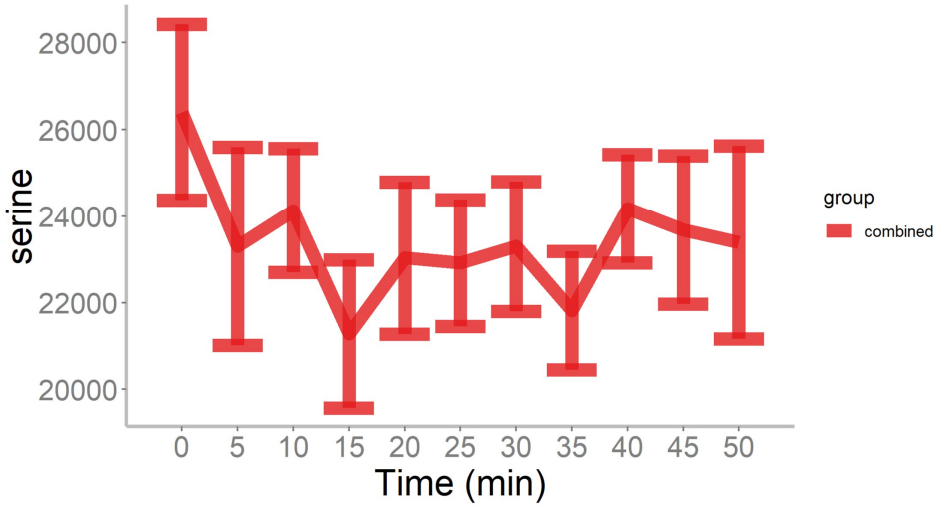

pyruvic acid
12000
11000
10000
9000
8000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

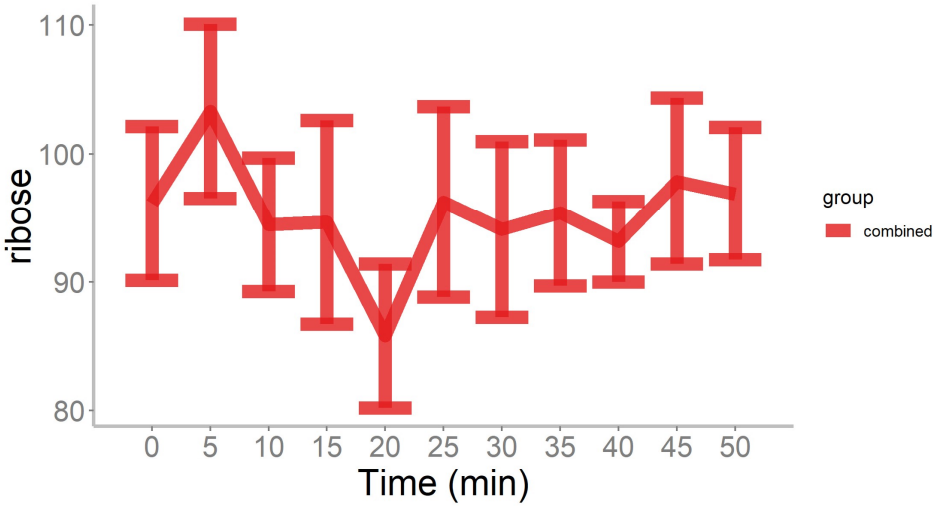

ribitol
1500
1400
1300
1200
1100
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

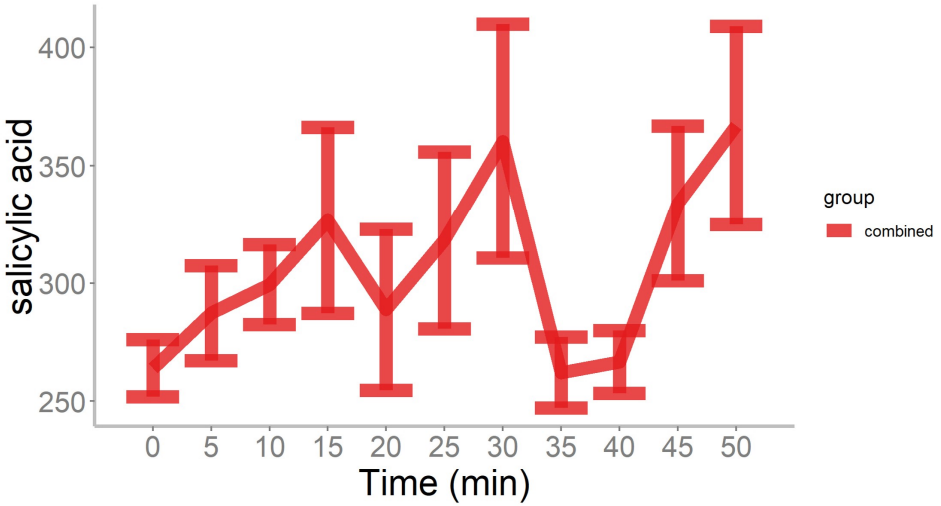

pyrrole-2-carboxylic acid
300
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


quinic acid
440
400
360
320
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


salicylaldehyde
310
290
270
250
230
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


serine
28000
26000
24000
22000
20000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


ribose
110
100
90
80
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


salicylic acid
400
350
300
250
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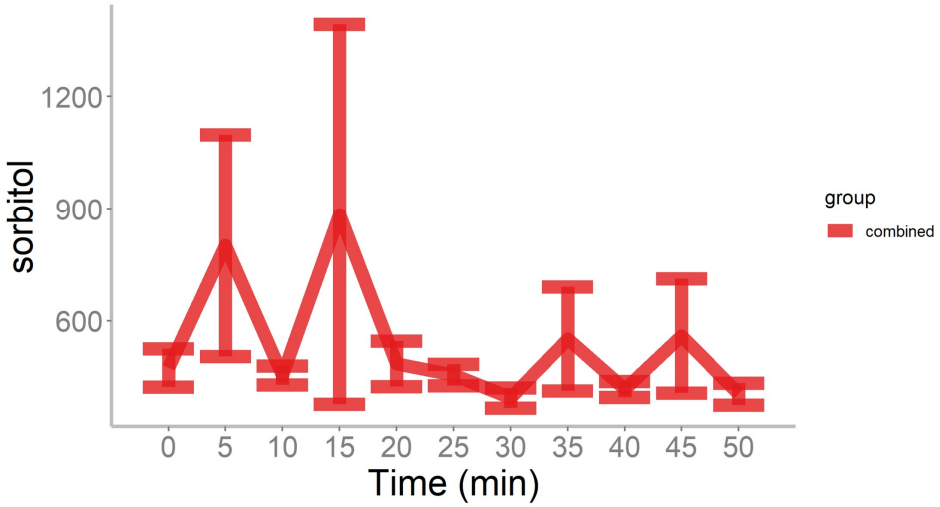
Time (min)
group
combined


sorbitol
1200
900
600
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Time (min)
group
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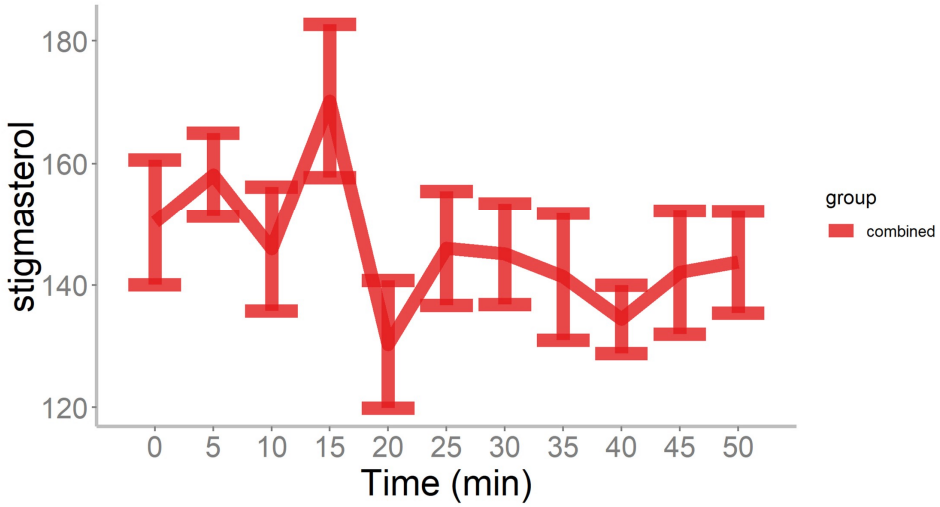
stigmasterol
180
160
140
120
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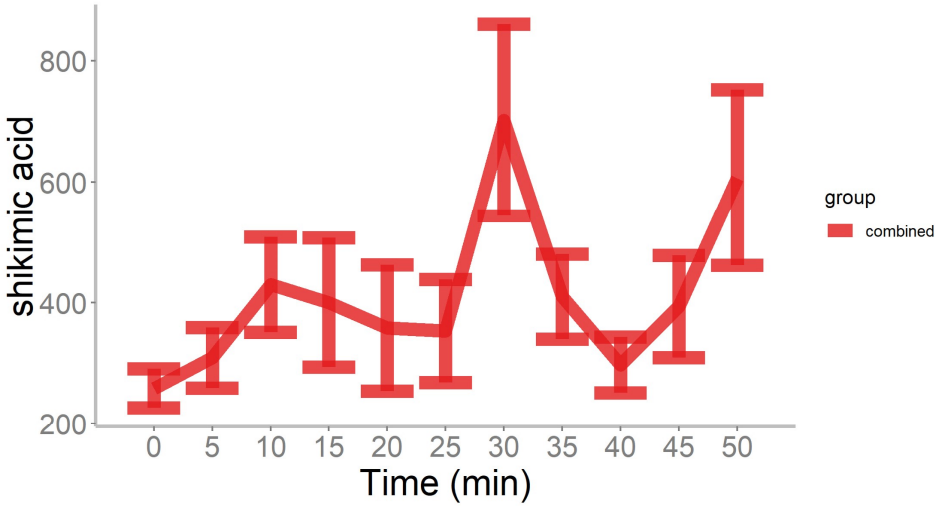
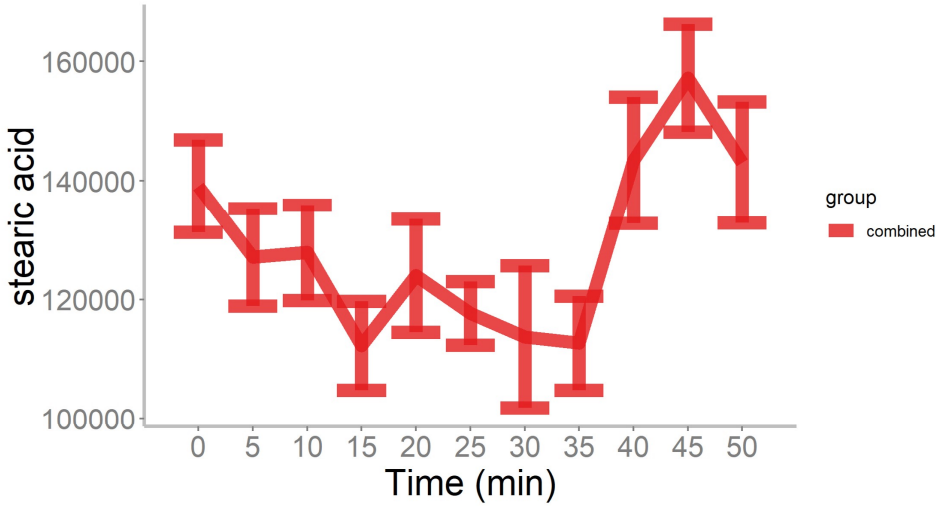
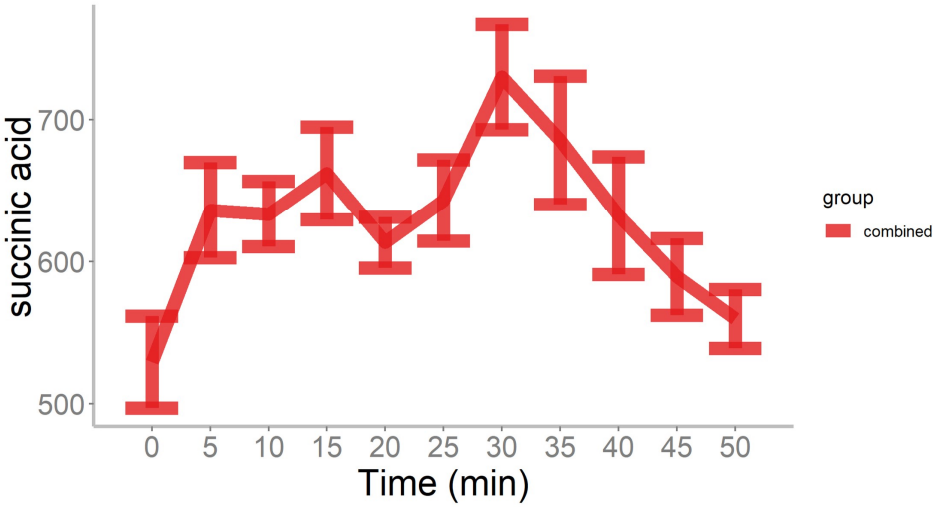
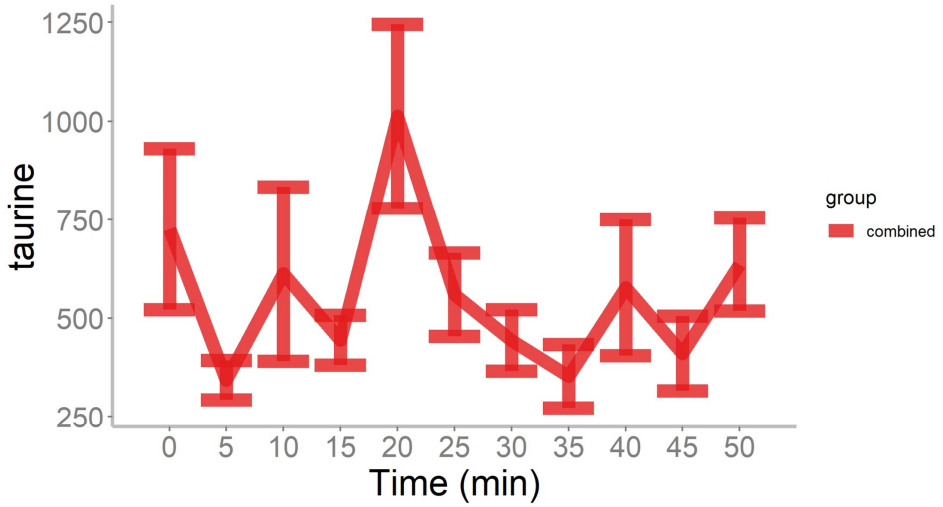
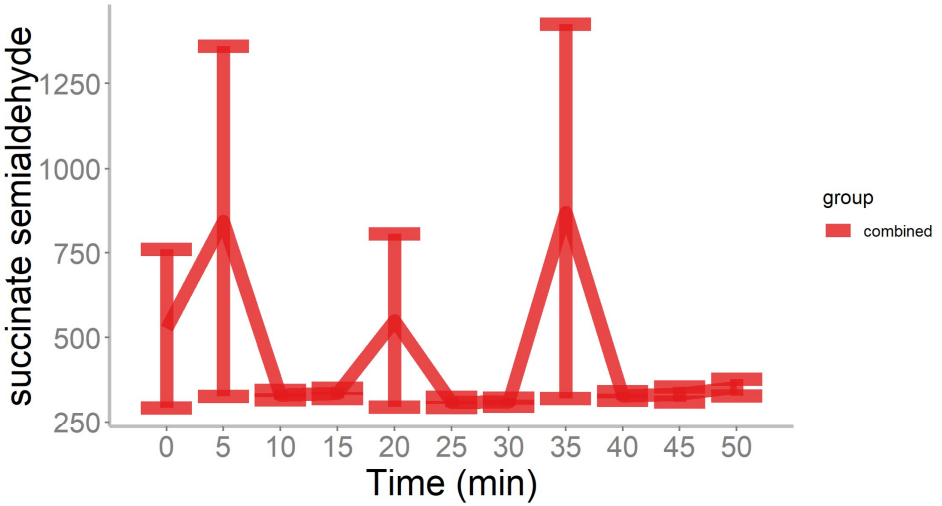
Time (min)
group
combined

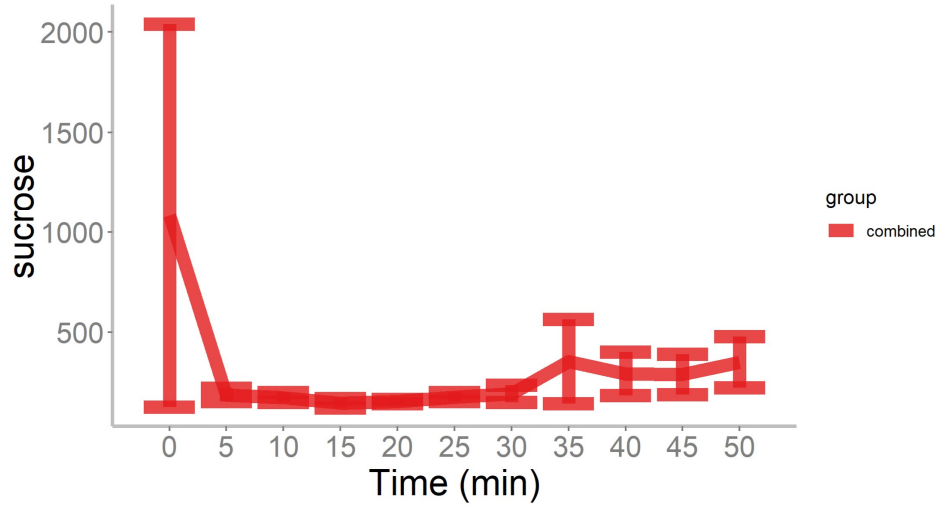

shikimic acid
800
600
400
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

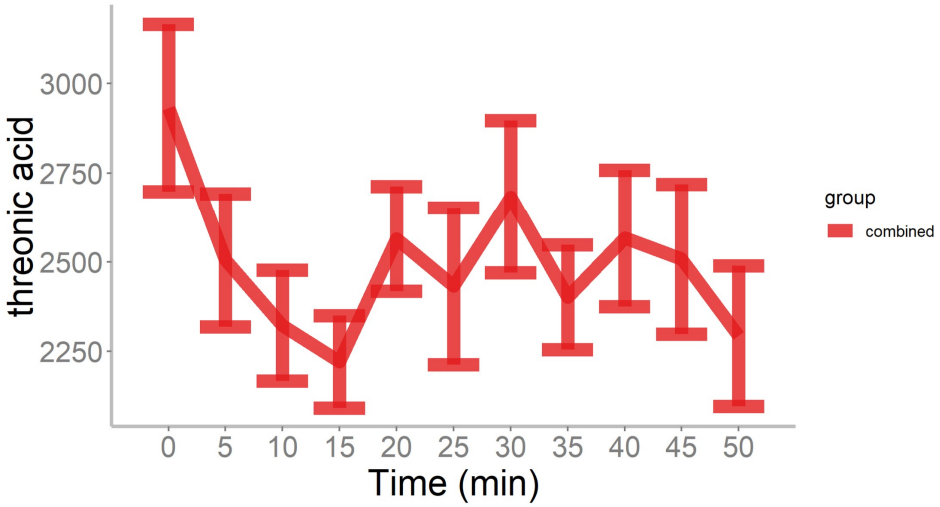

stearic acid
160000
140000
120000
100000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

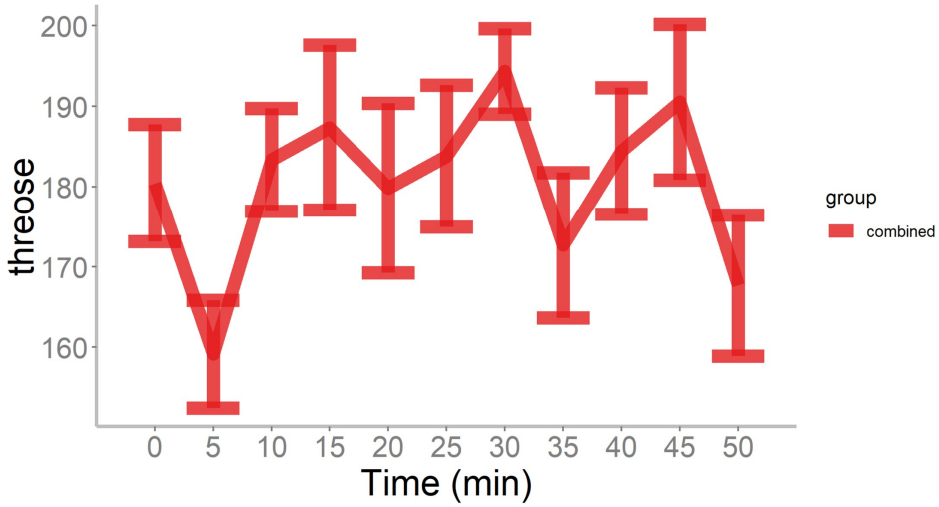

succinic acid
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

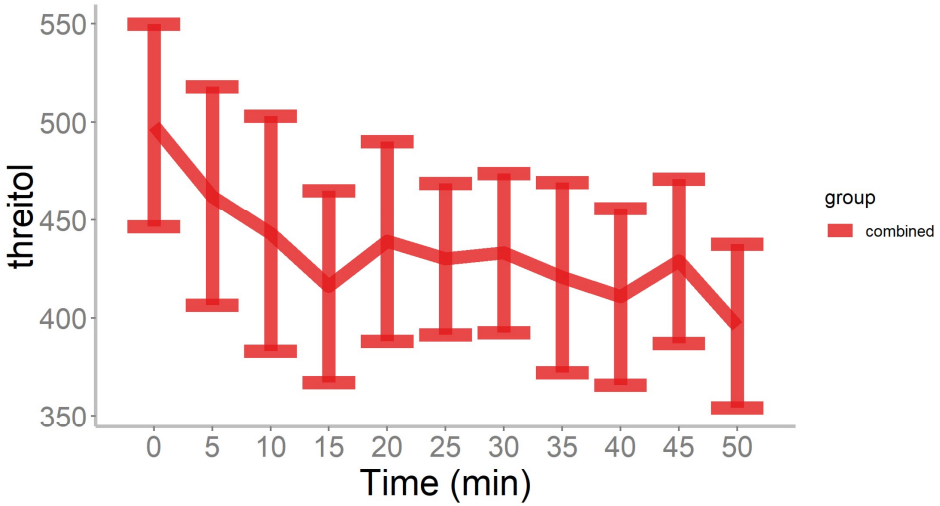

taurine
1250
1000
750
500
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

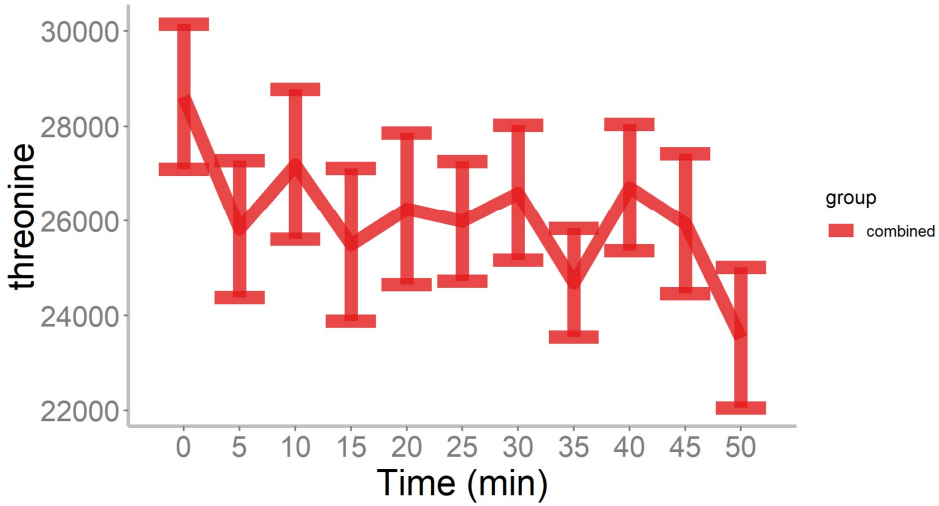

succinate semialdehyde
1250
1000
750
500
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

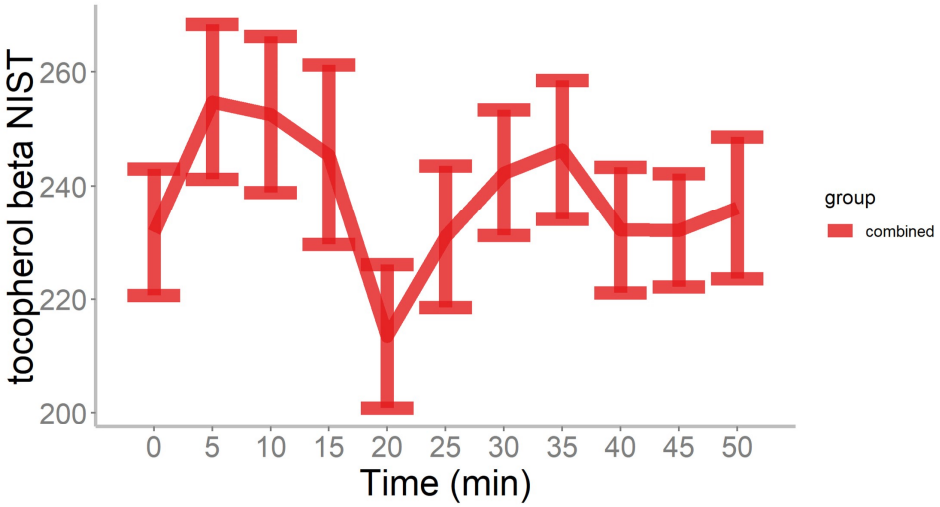

sucrose
2000
1500
1000
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

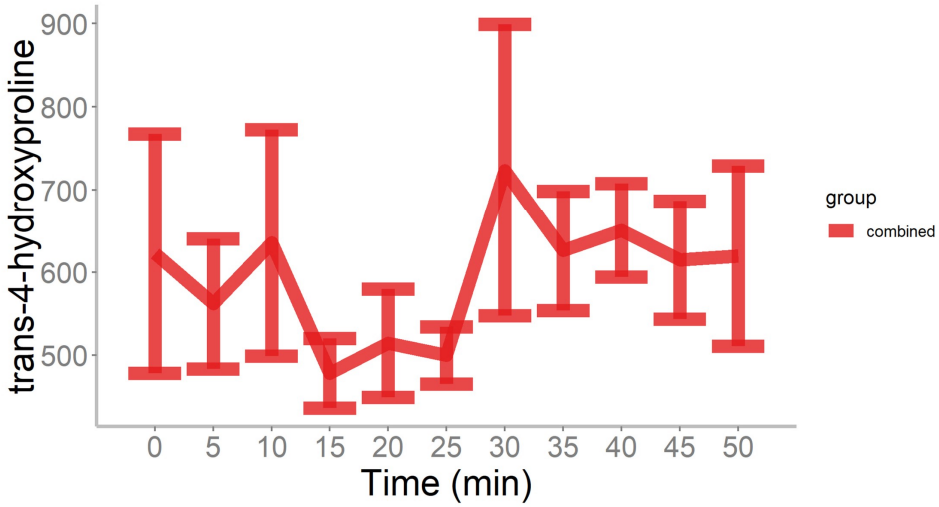

threonic acid
3000
2750
2500
2250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

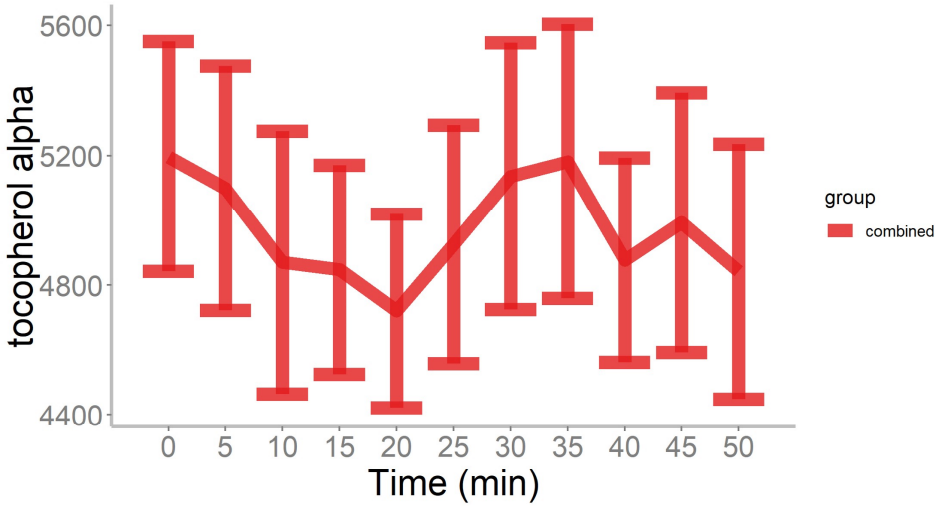

threose
200
190
180
170
160
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

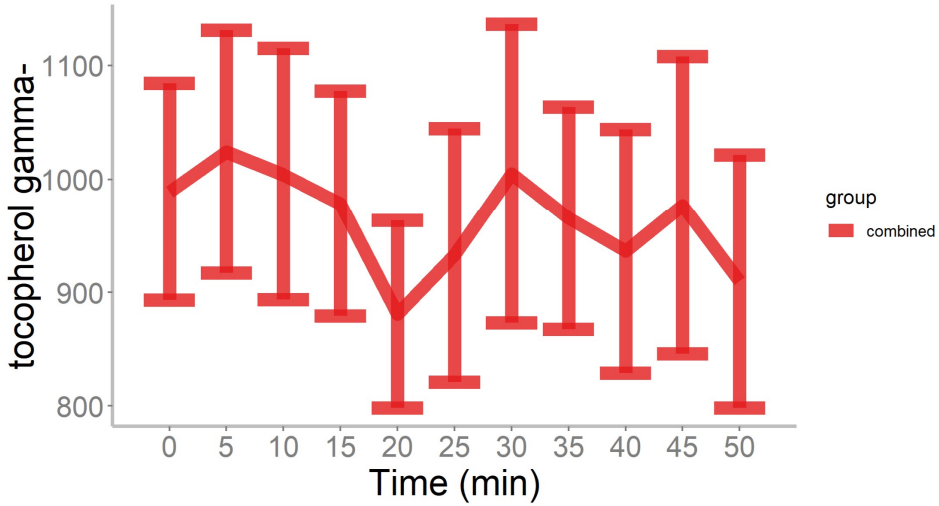

threitol
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

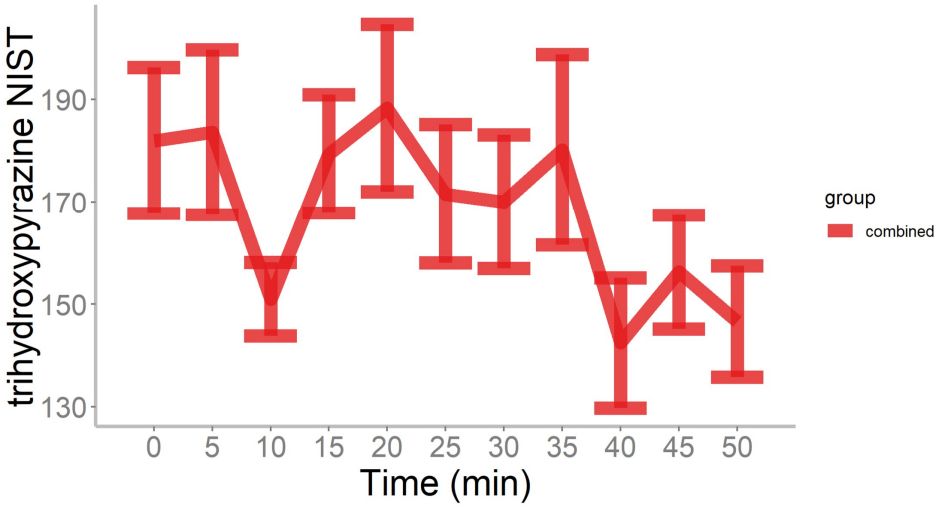

threonine
30000
28000
26000
24000
22000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

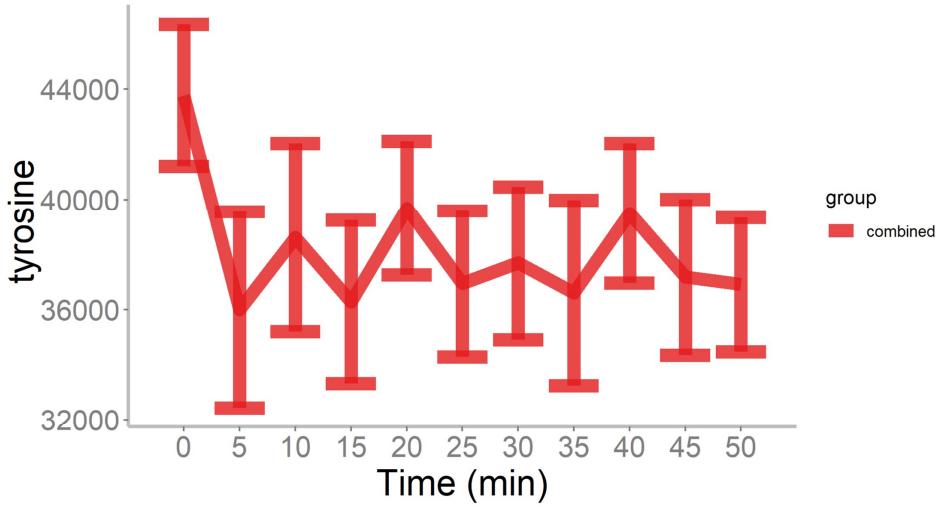

tocopherol beta NIST
260
240
220
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

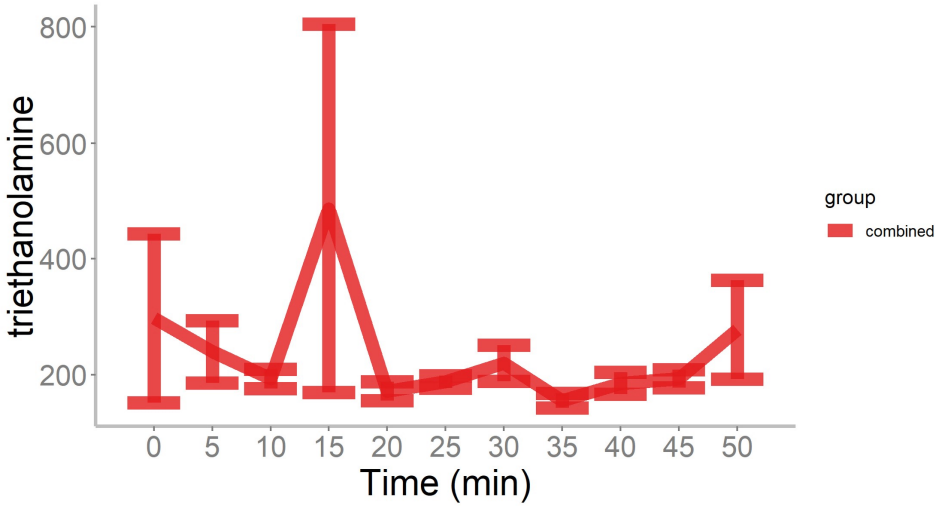

trans-4-hydroxyproline
900
800
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

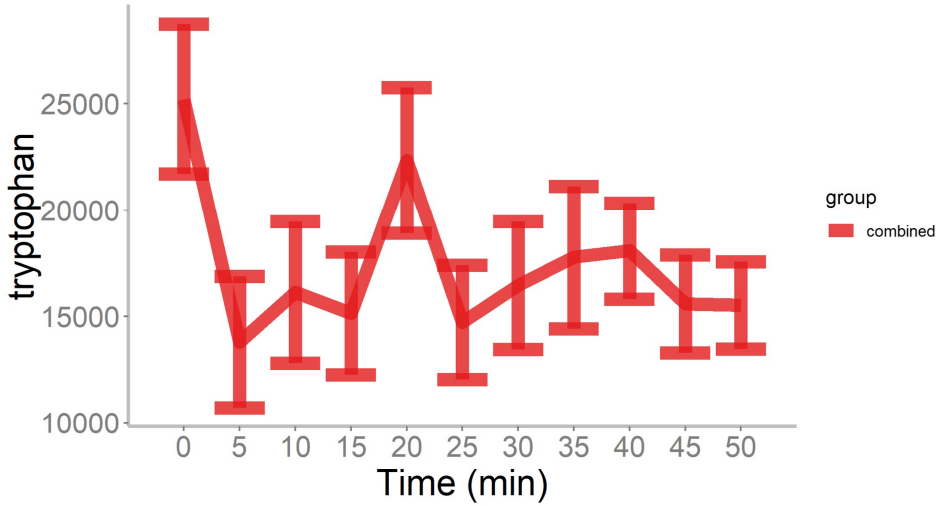

tocopherol alpha
5600
5200
4800
4400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

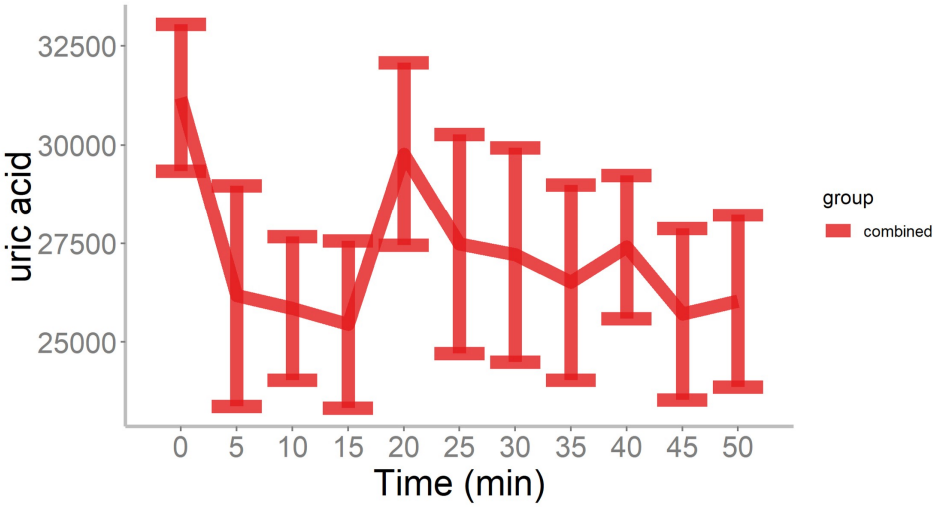

tocopherol gamma-
1100
1000
900
800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

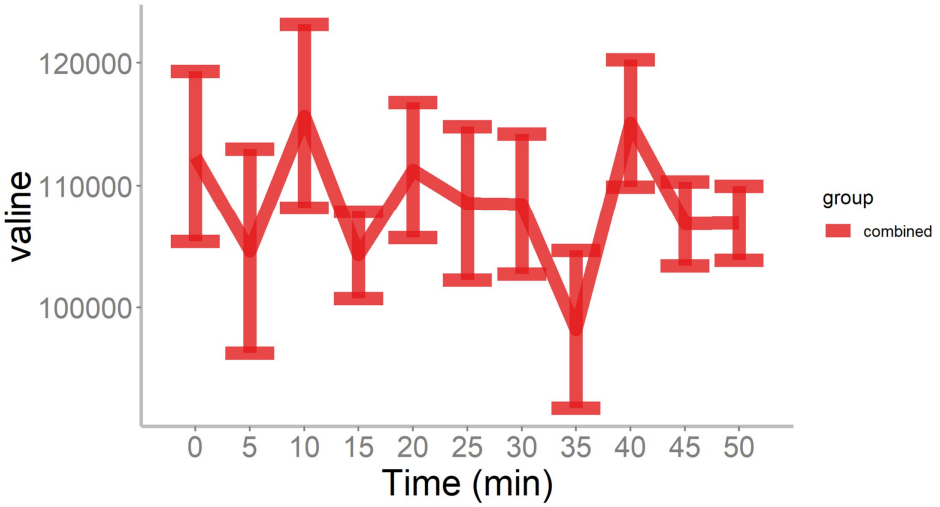

trihydroxypyrazine NIST
190
170
150
130
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

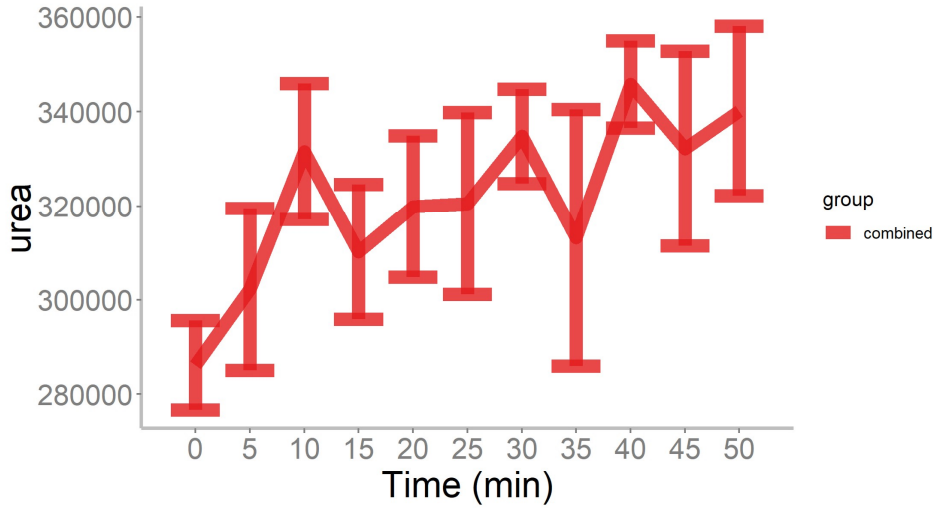

tyrosine
44000
40000
36000
32000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

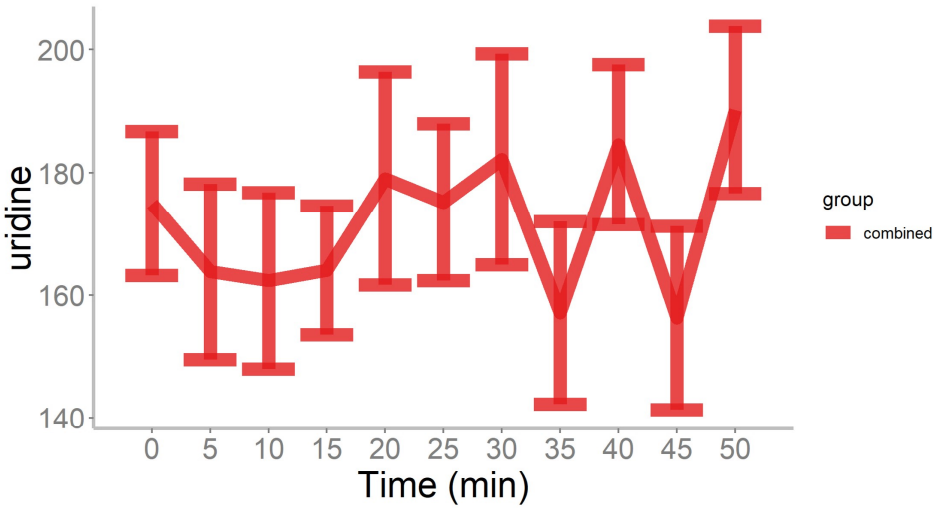

triethanolamine
800
600
400
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

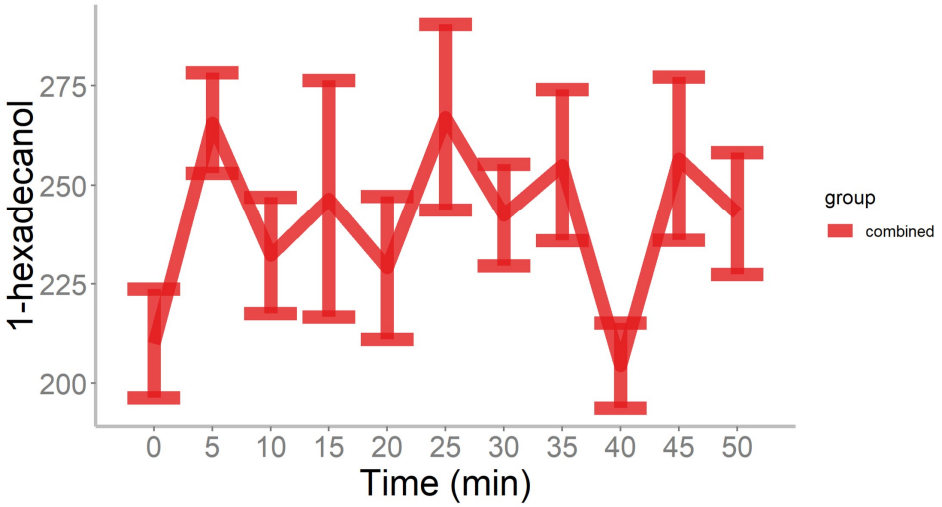

tryptophan
25000
20000
15000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

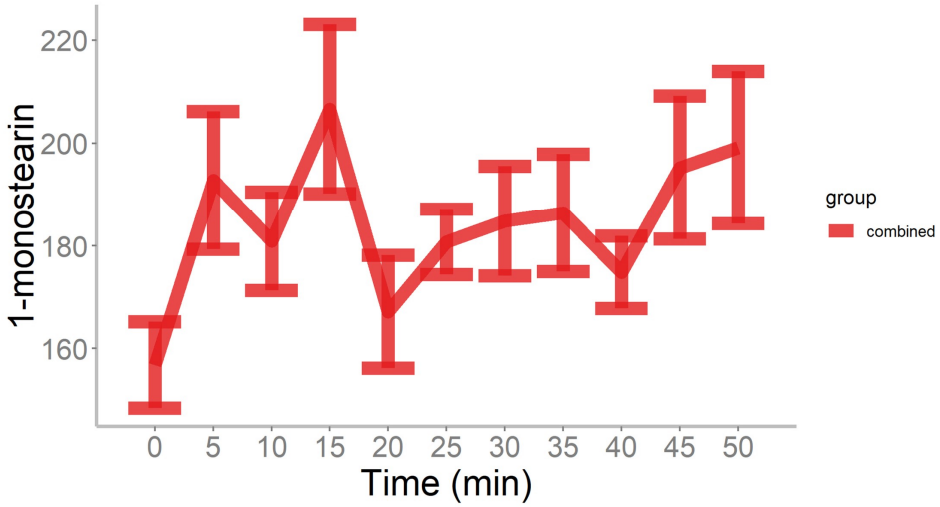

uric acid
32500
30000
27500
25000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

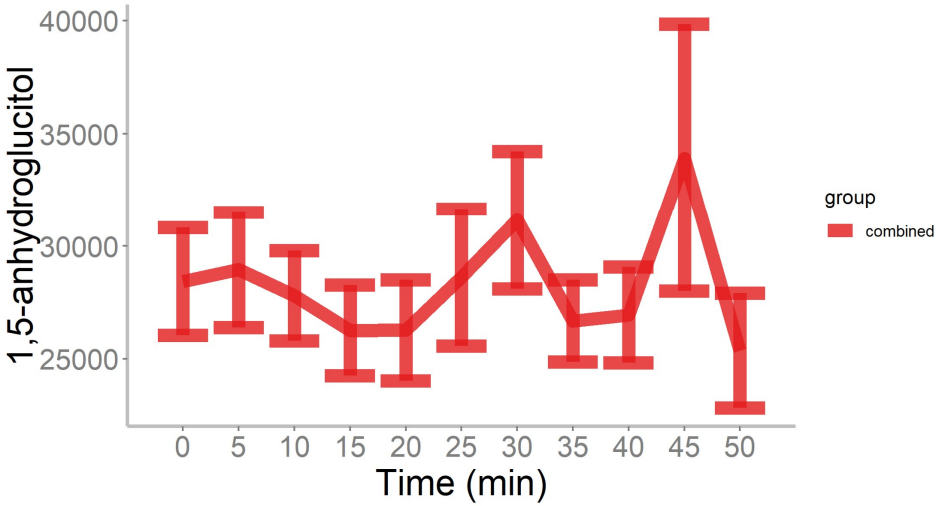

valine
120000
110000
100000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

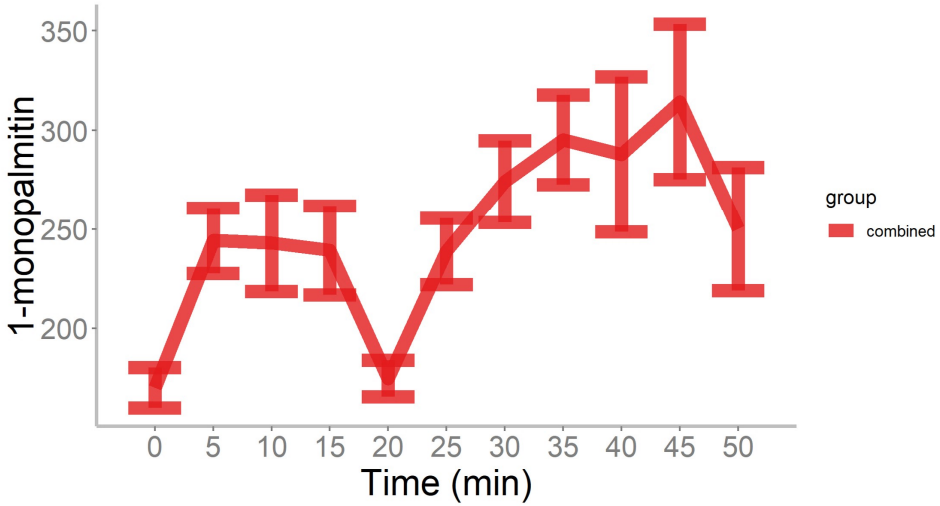

urea
360000
340000
320000
300000
280000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

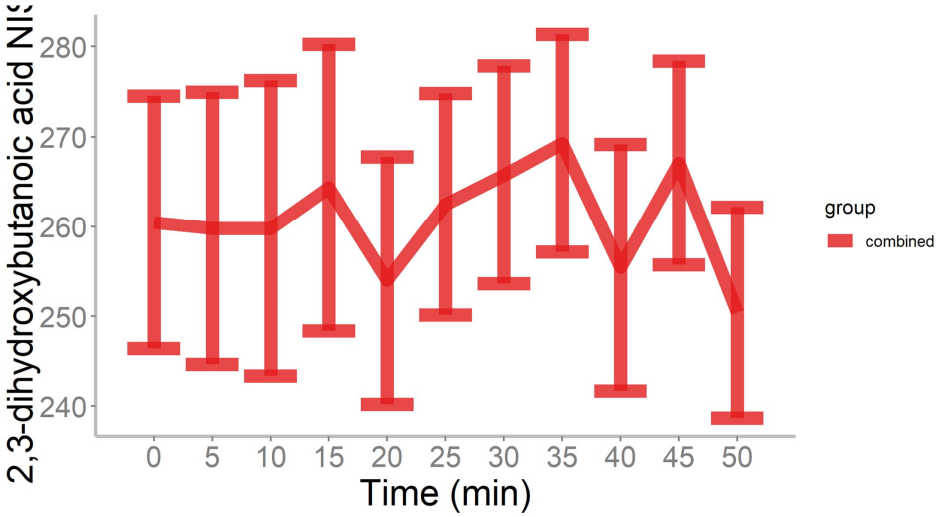

uridine
200
180
160
140
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

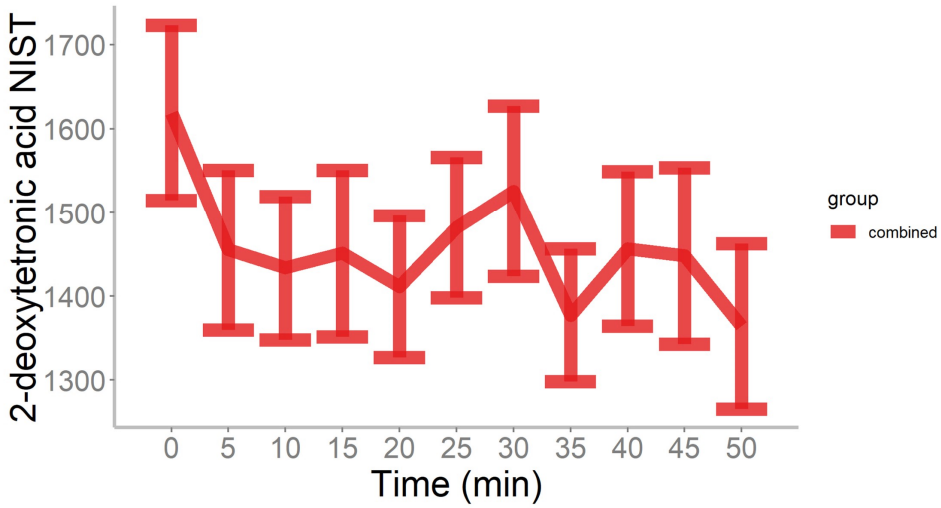

1-hexadecanol
275
250
225
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

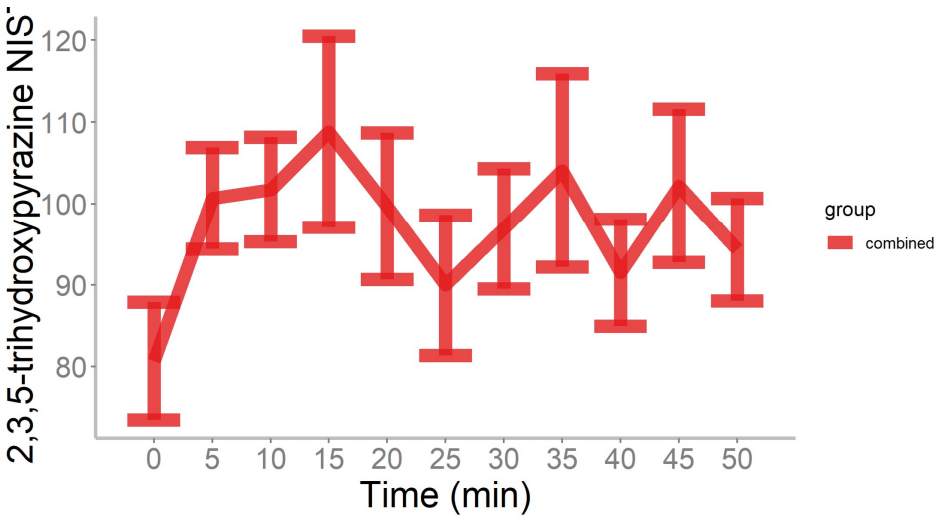

1-monostearin
220
200
180
160
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

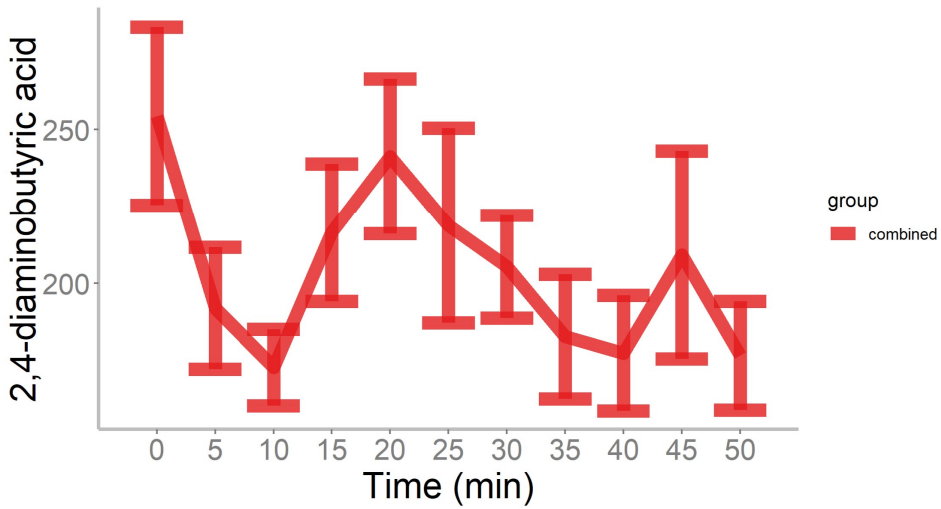

1,5-anhydroglucitol
40000
35000
30000
25000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

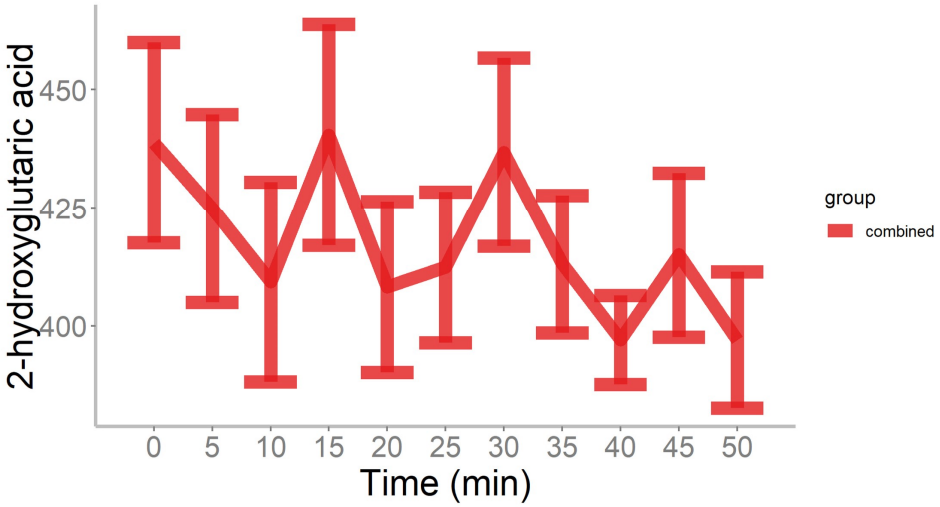

1-monopalmitin
350
300
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

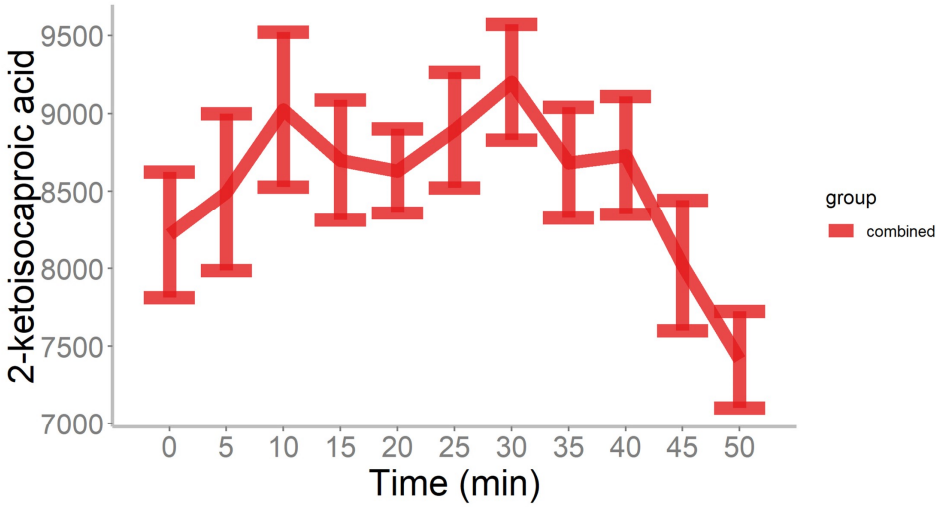

2,3-dihydroxybutanoic acid NIS
280
270
260
250
240
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

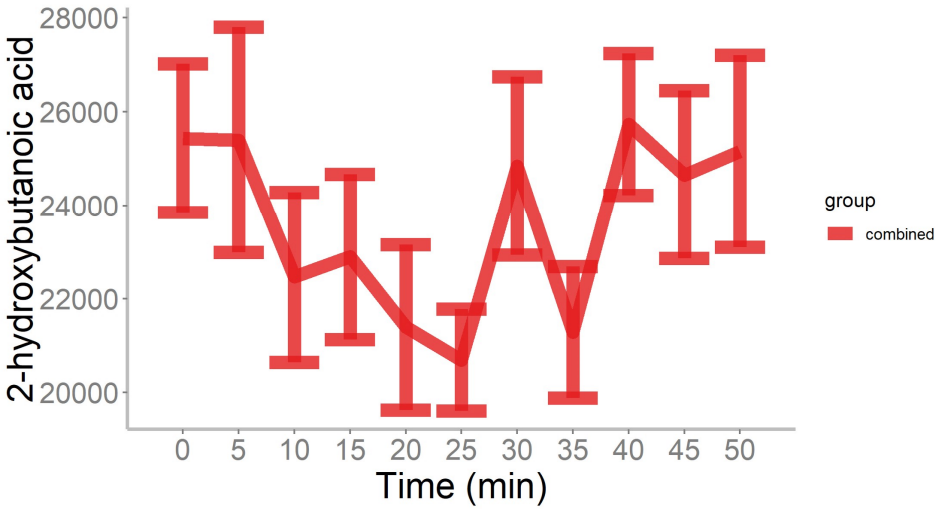

2-deoxytetronic acid NIST
1700
1600
1500
1400
1300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

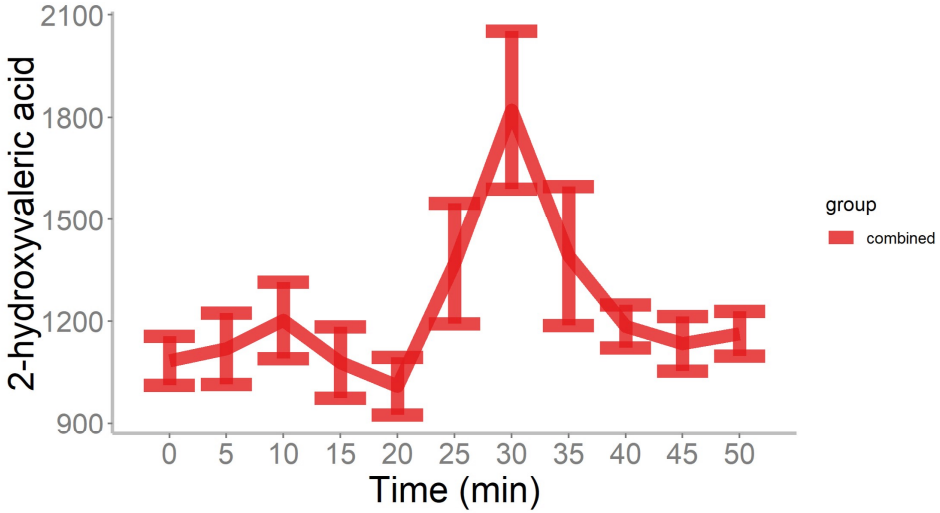

2,3,5-trihydroxypyrazine NIS
120
110
100
90
80
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

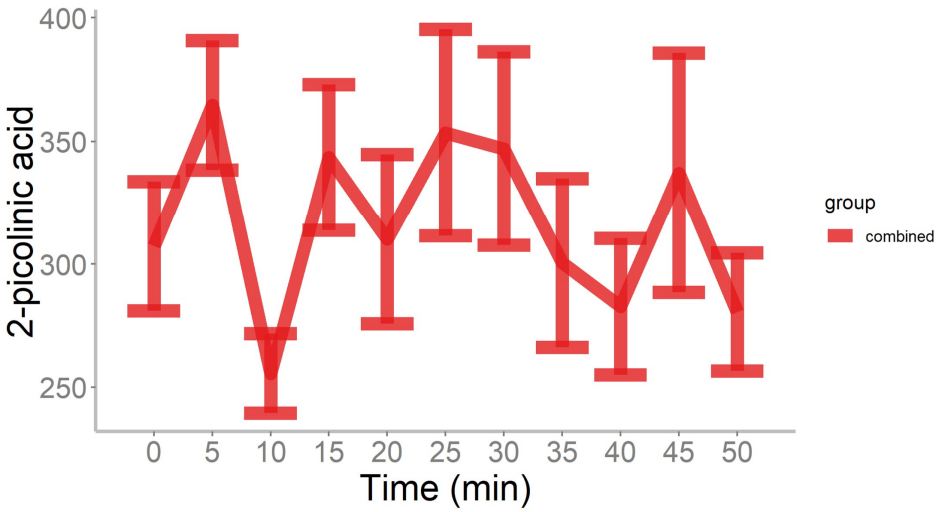

2,4-diaminobutyric acid
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

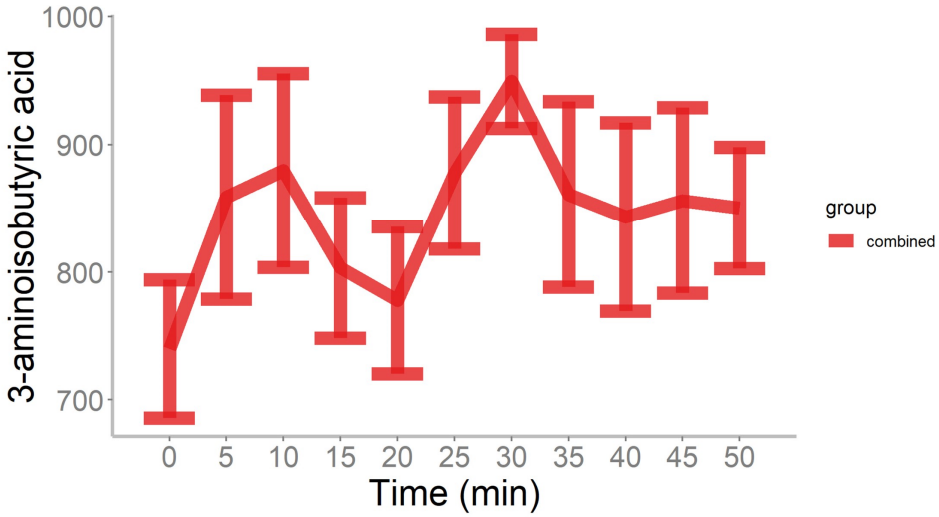

2-hydroxyglutaric acid
450
425
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

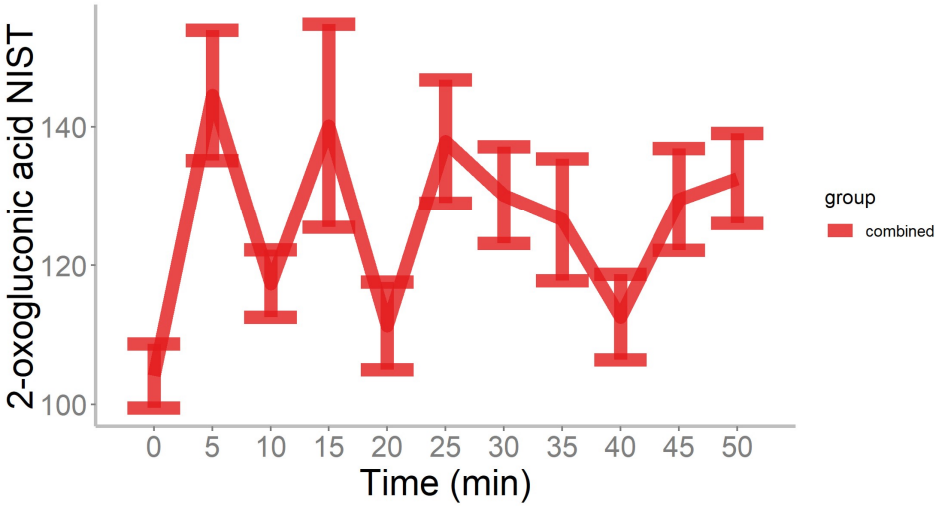

2-ketoisocaproic acid
9500
9000
8500
8000
7500
7000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

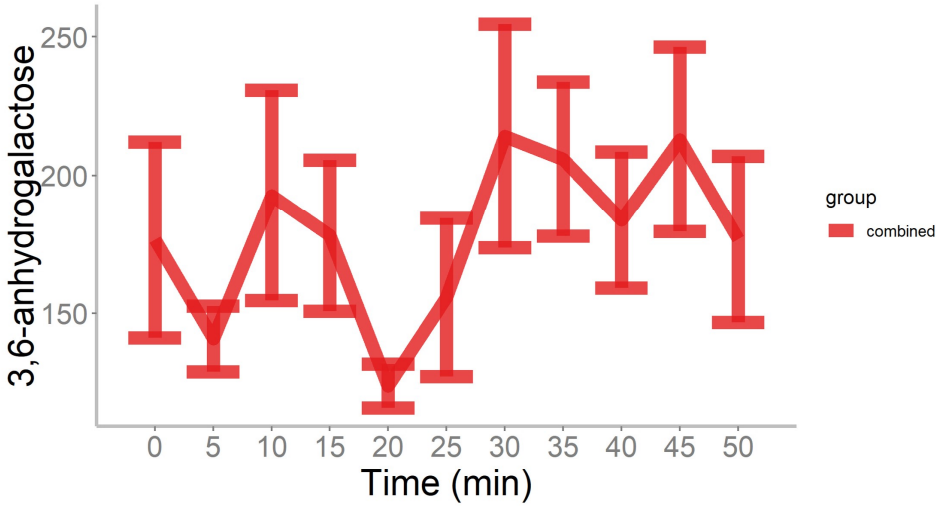

2-hydroxybutanoic acid
28000
26000
24000
22000
20000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

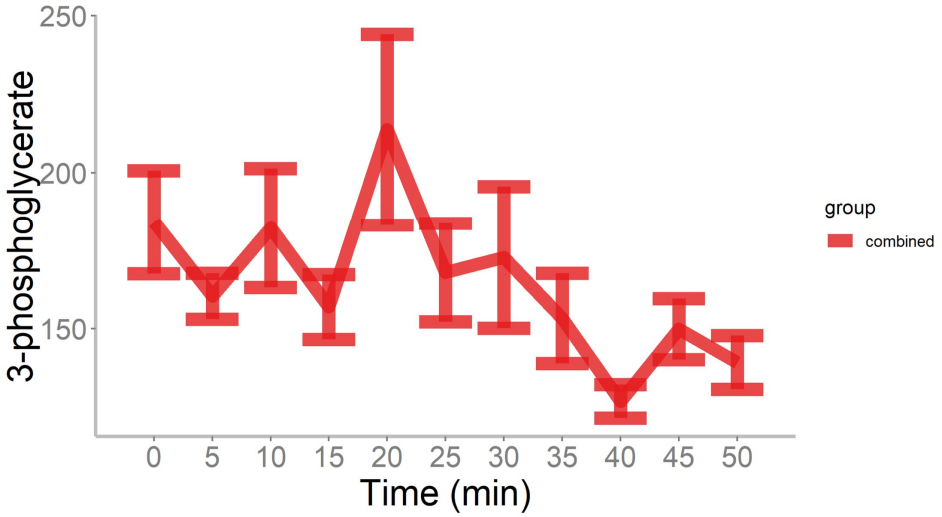

2-hydroxyvaleric acid
2100
1800
1500
1200
900
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

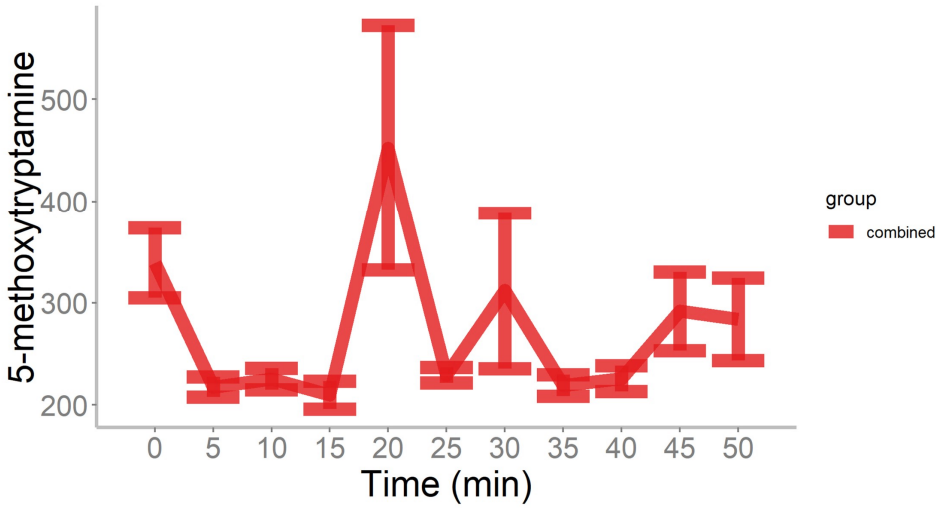

2-picolinic acid
400
350
300
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

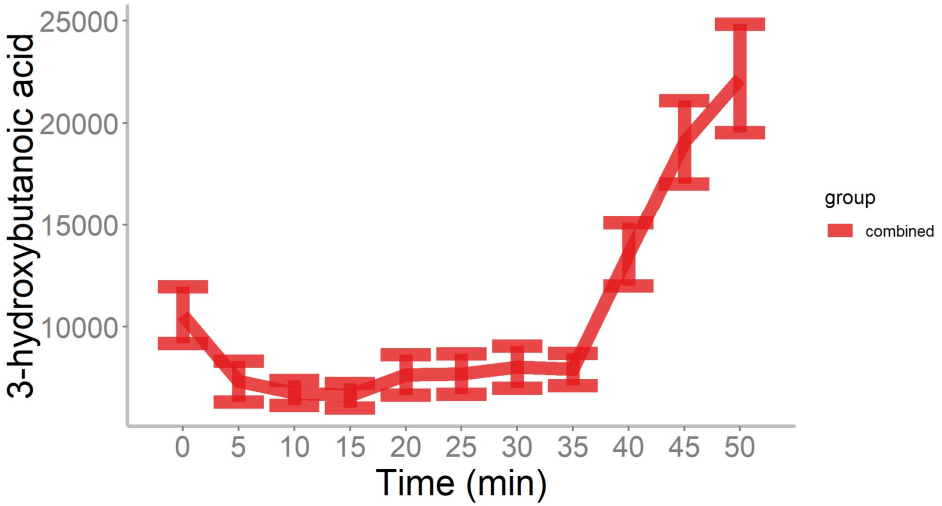

3-aminoisobutyric acid
1000
900
800
700
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

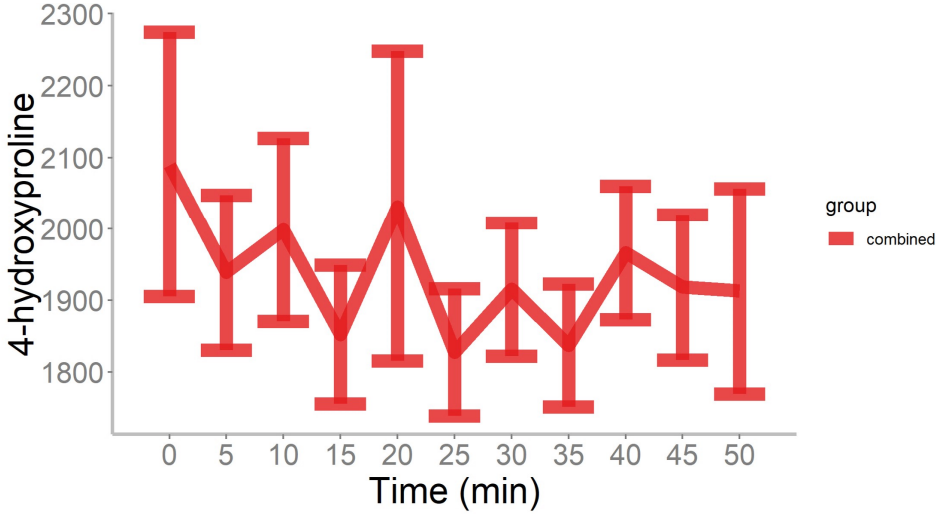

2-oxogluconic acid NIST
140
120
100
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

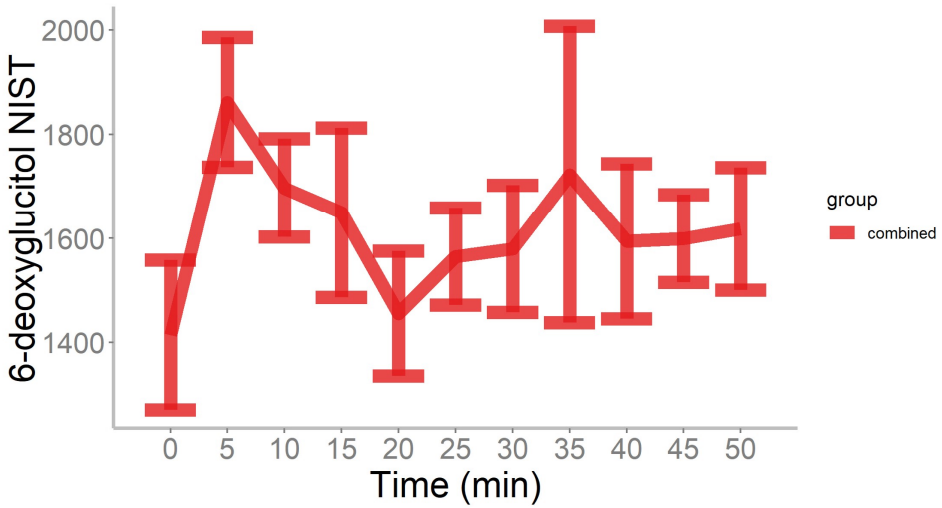

3,6-anhydrogalactose
250
200
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

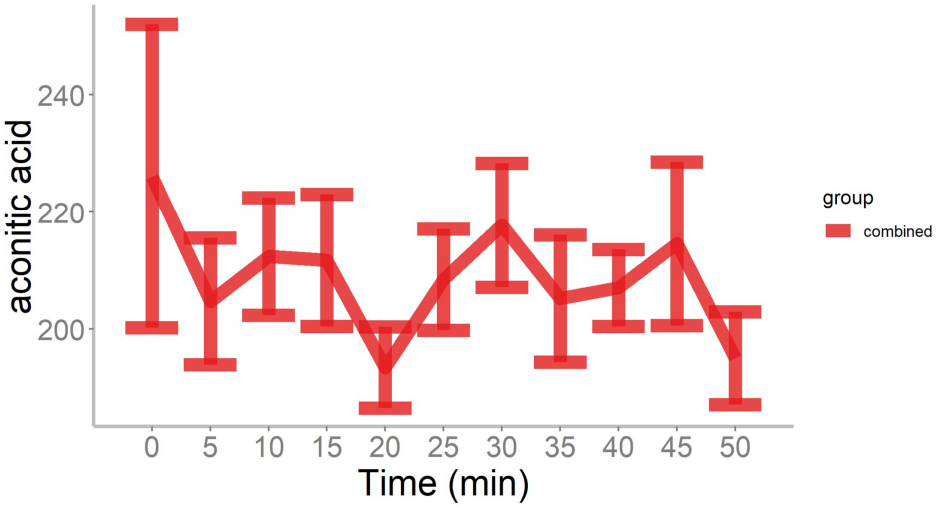

3-phosphoglycerate
250
200
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

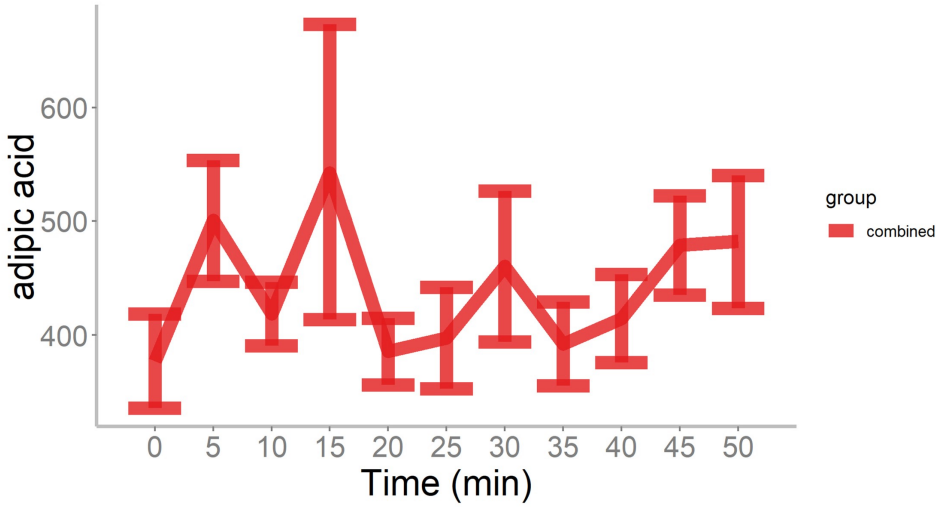

5-methoxytryptamine
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


3-hydroxybutanoic acid
25000
20000
15000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


4-hydroxyproline
2300
2200
2100
2000
1900
1800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


6-deoxyglucitol NIST
2000
1800
1600
1400
0
5
10
15
20
25
30
35
40
45
50
Time (min)
group
combined


aconitic acid
240
220
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


adipic acid
600
500
400
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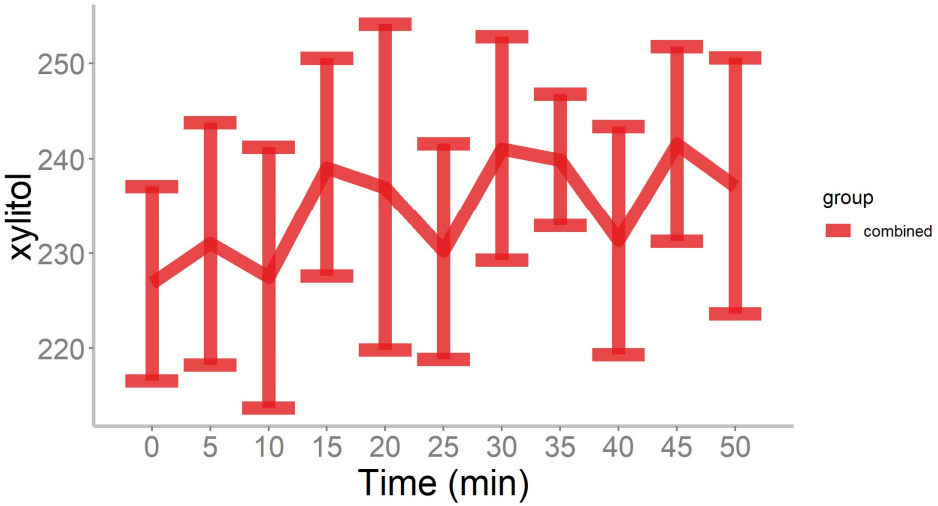
Time (min)
group
combined


xylitol
250
240
230
220
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Time (min)
group
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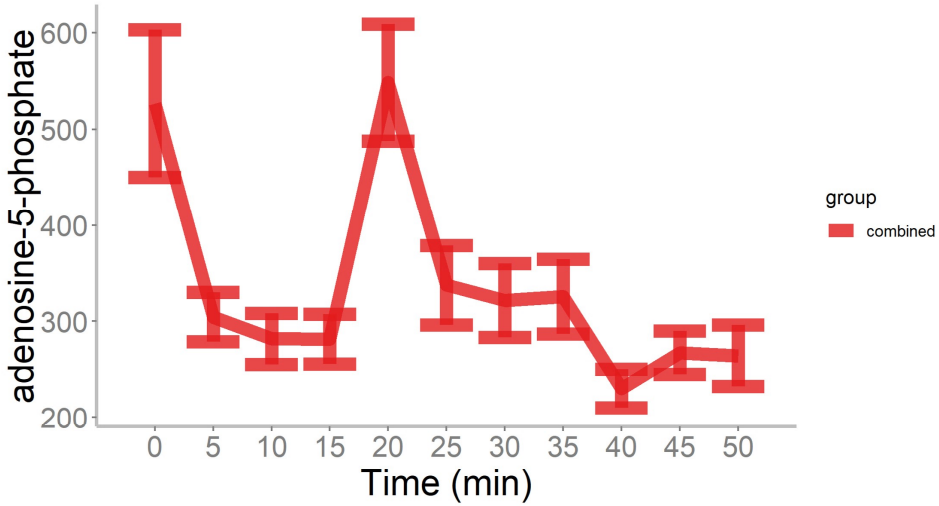
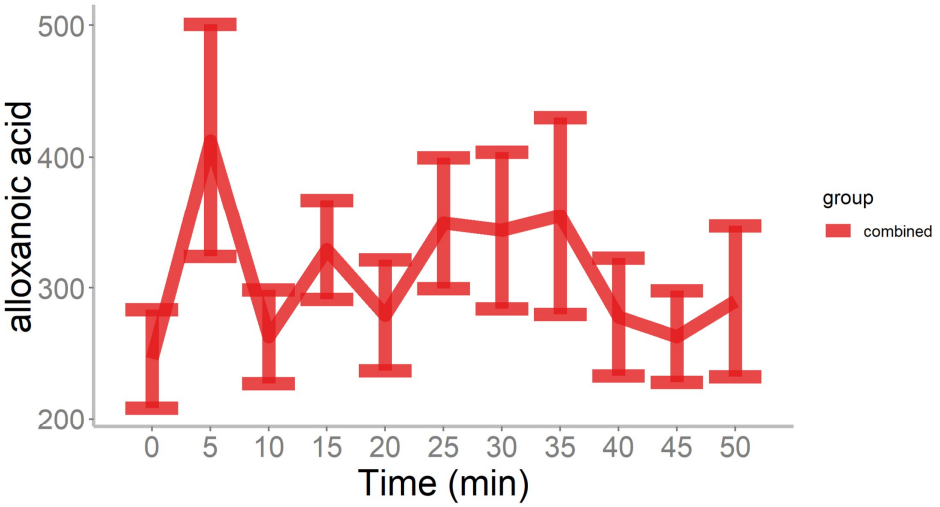
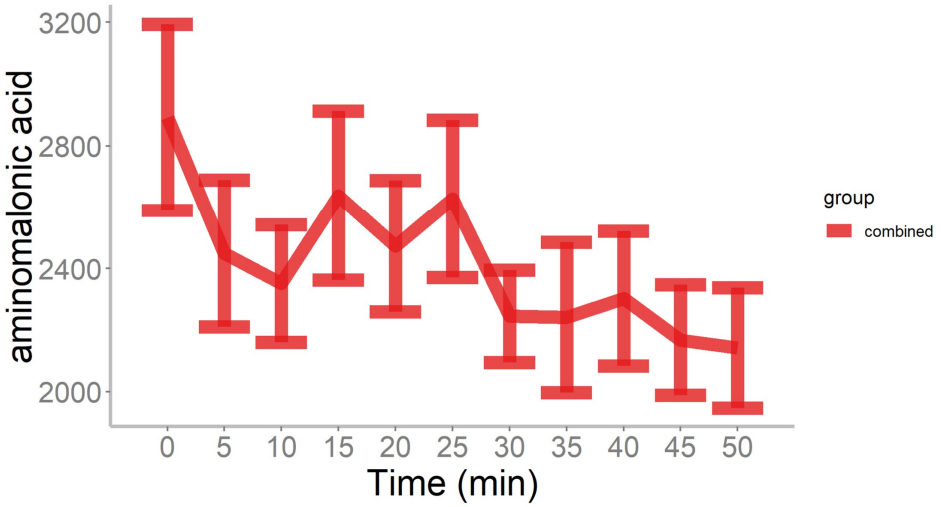
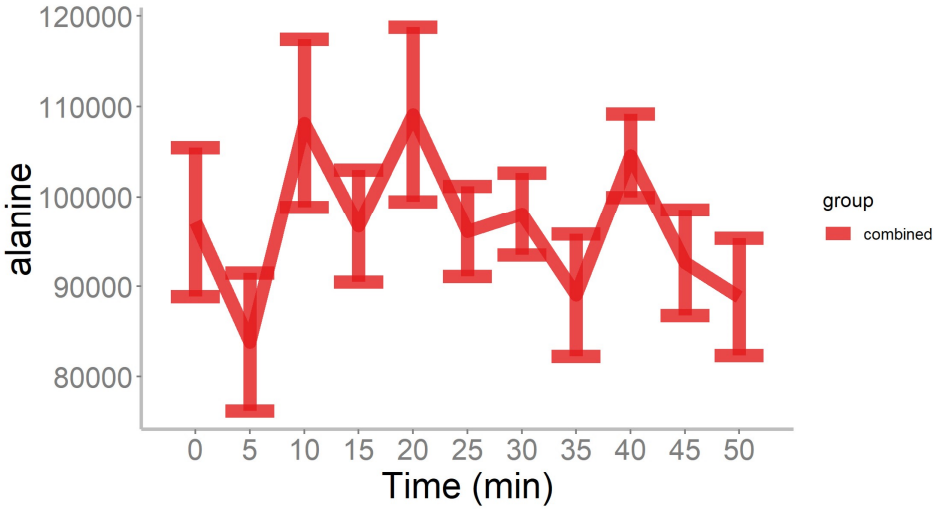

adenosine-5-phosphate
600
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


alloxanoic acid
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


aminomalonic acid
3200
2800
2400
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


alanine
120000
110000
100000
90000
80000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
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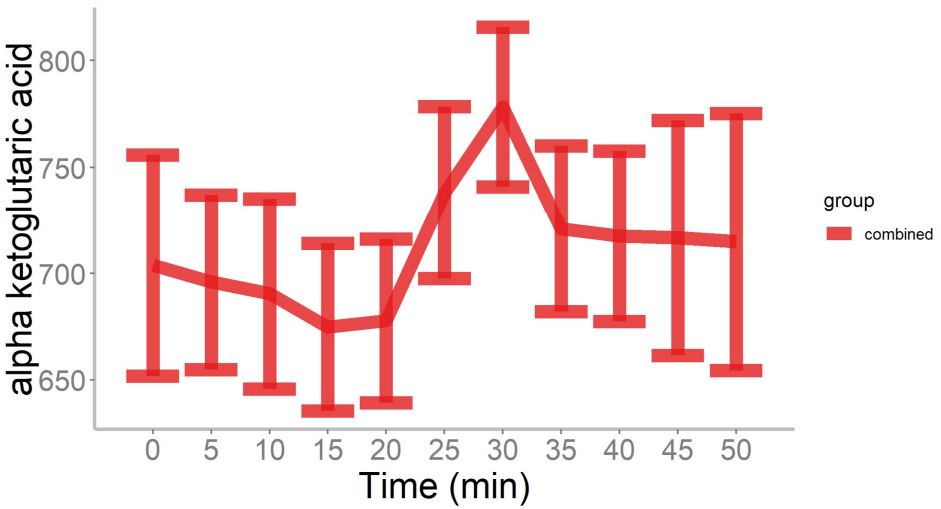
alpha ketoglutaric acid
800
750
700
650
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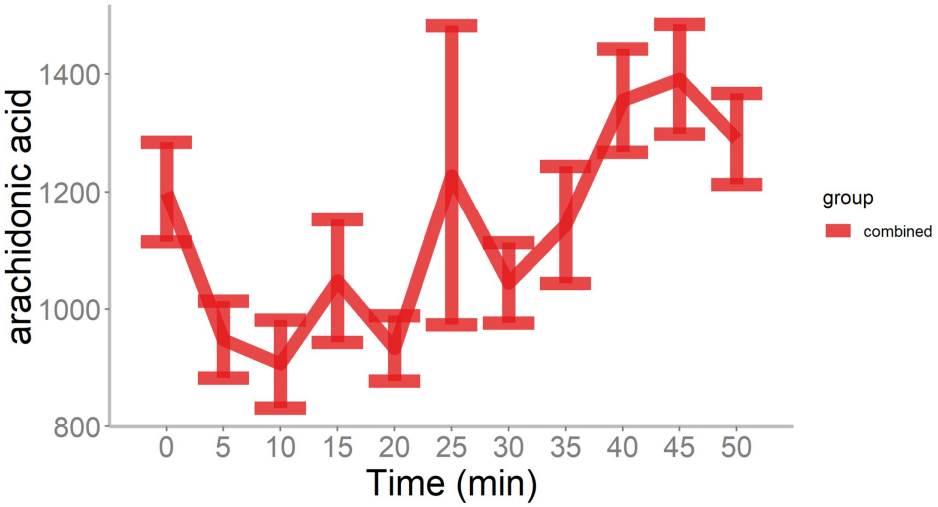
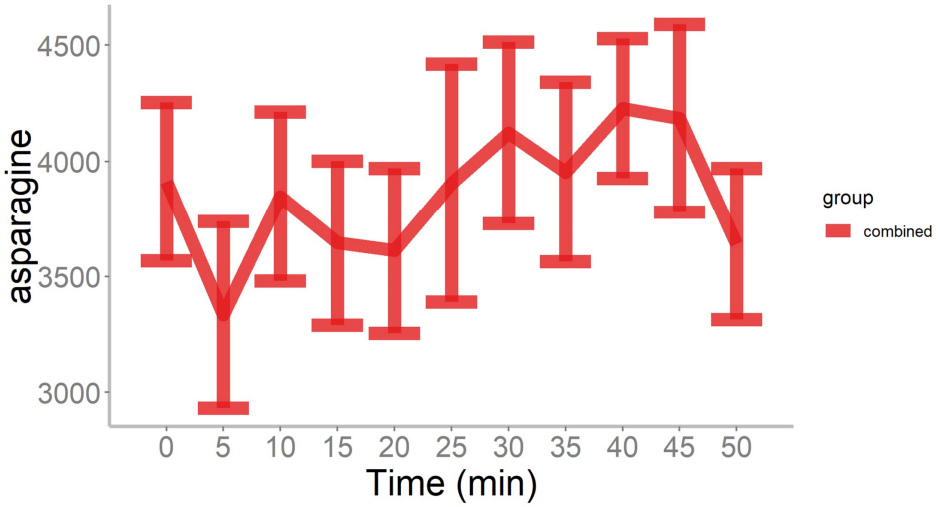
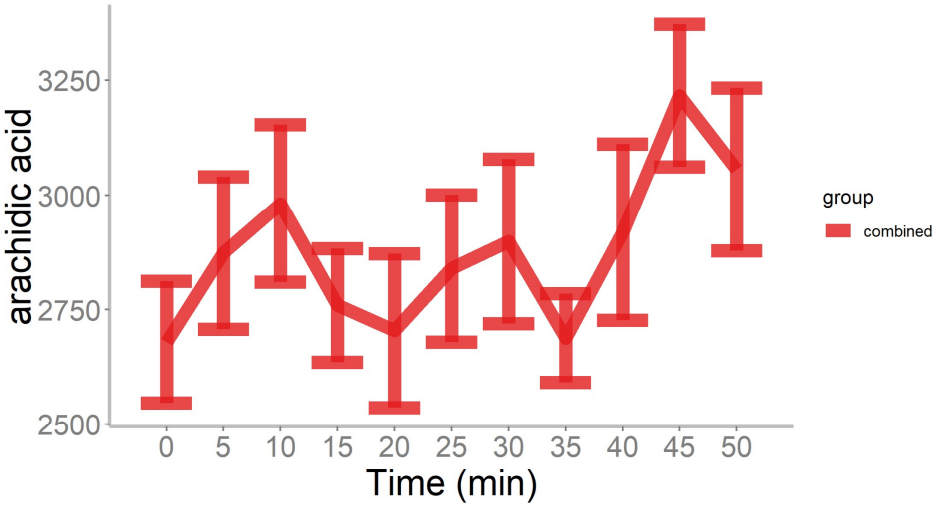
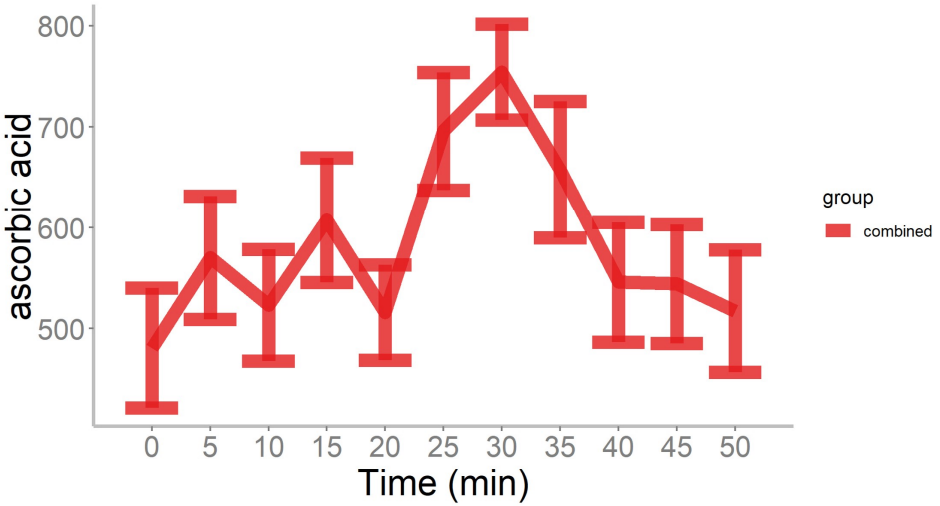
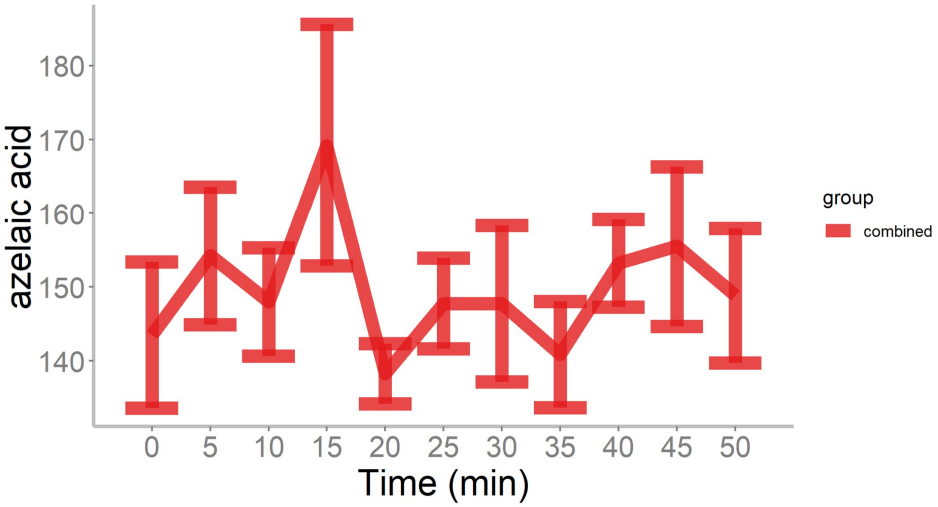
Time (min)
group
combined

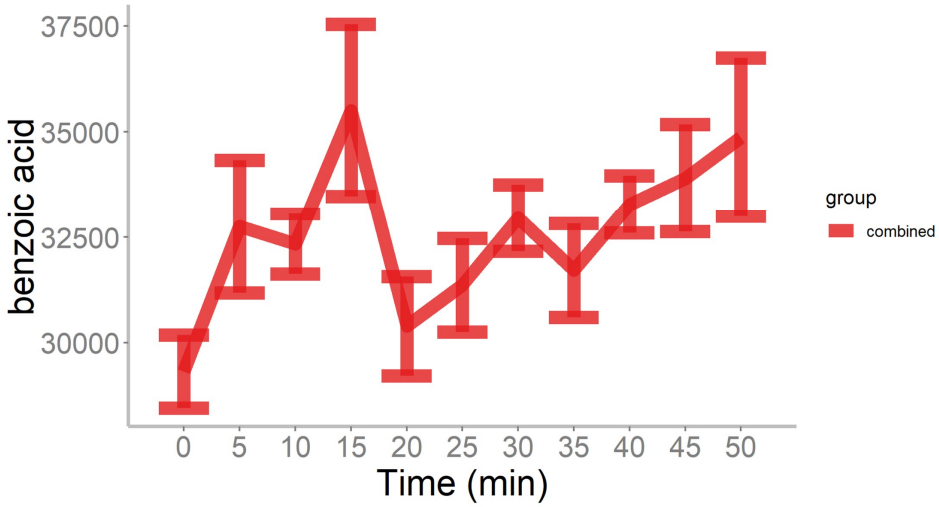

arachidonic acid
1400
1200
1000
800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

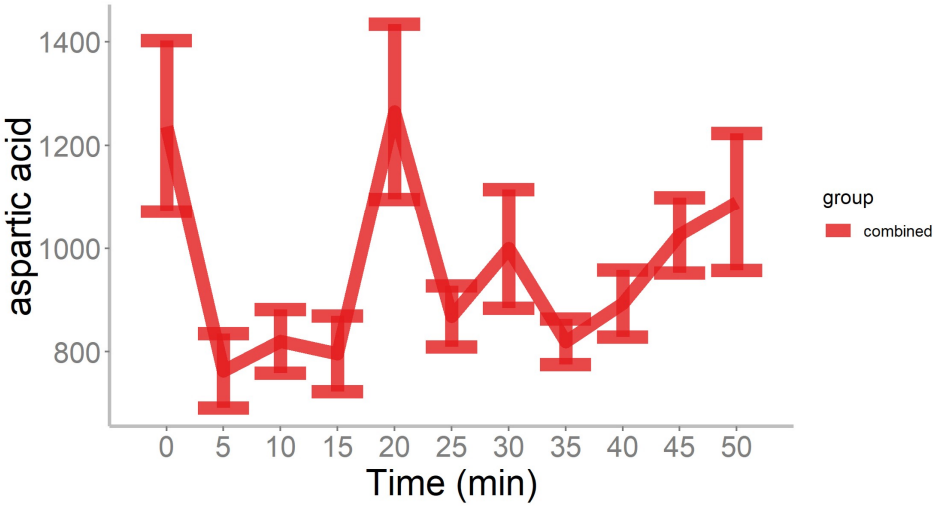

asparagine
4500
4000
3500
3000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

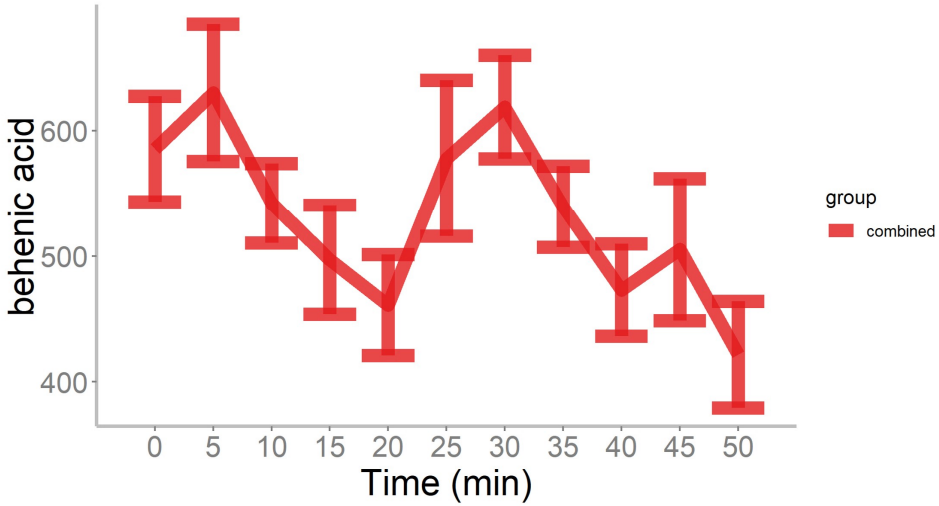

arachidic acid
3250
3000
2750
2500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

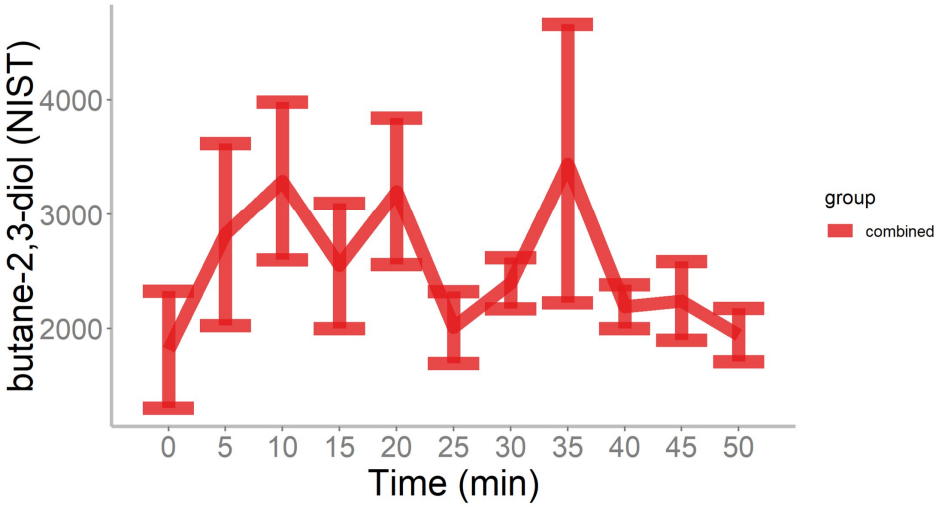

ascorbic acid
800
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

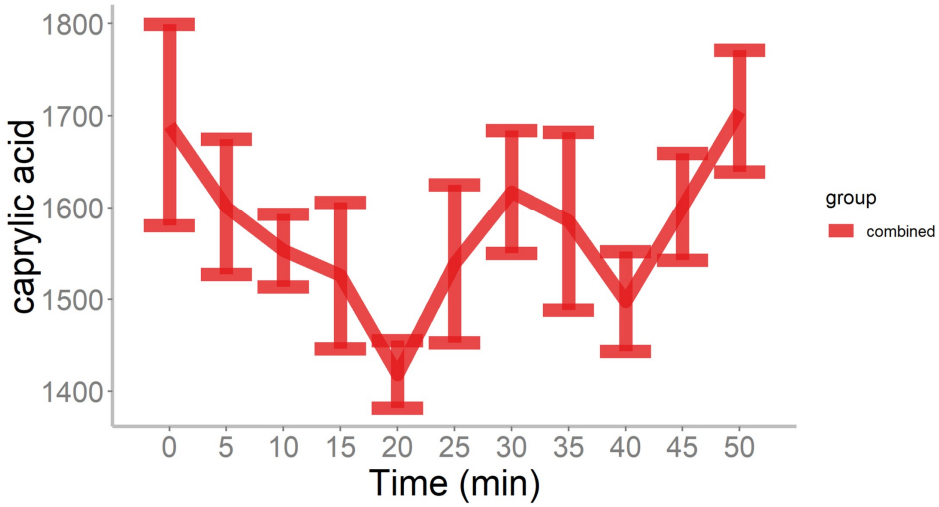

azelaic acid
180
170
160
150
140
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

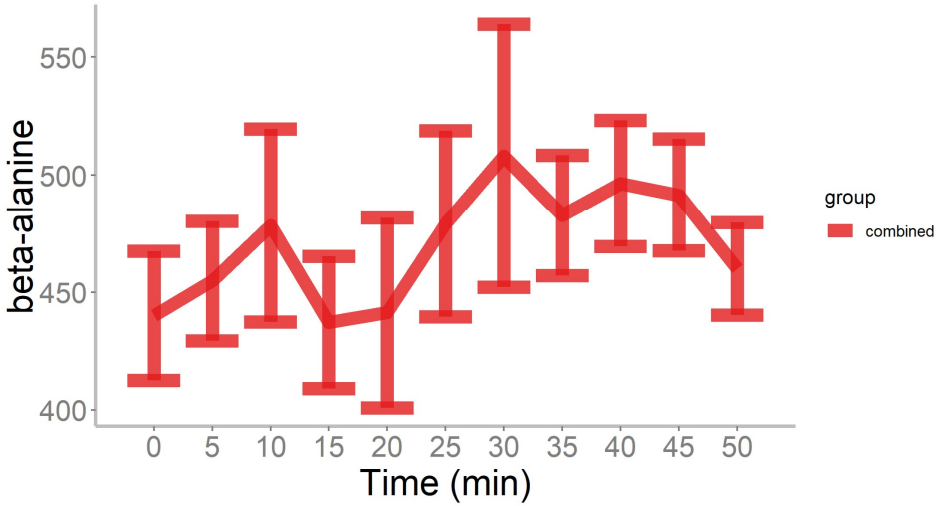

benzoic acid
37500
35000
32500
30000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

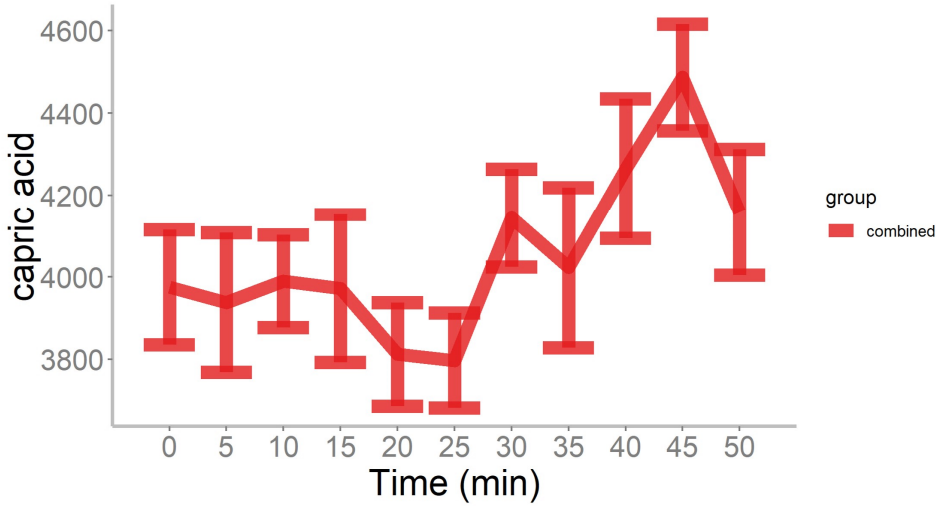

aspartic acid
1400
1200
1000
800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

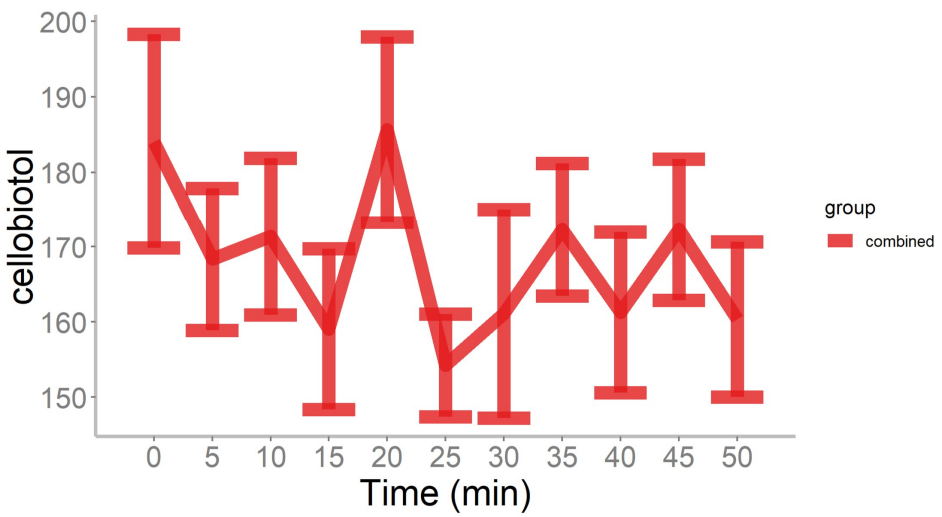

behenic acid
600
500
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

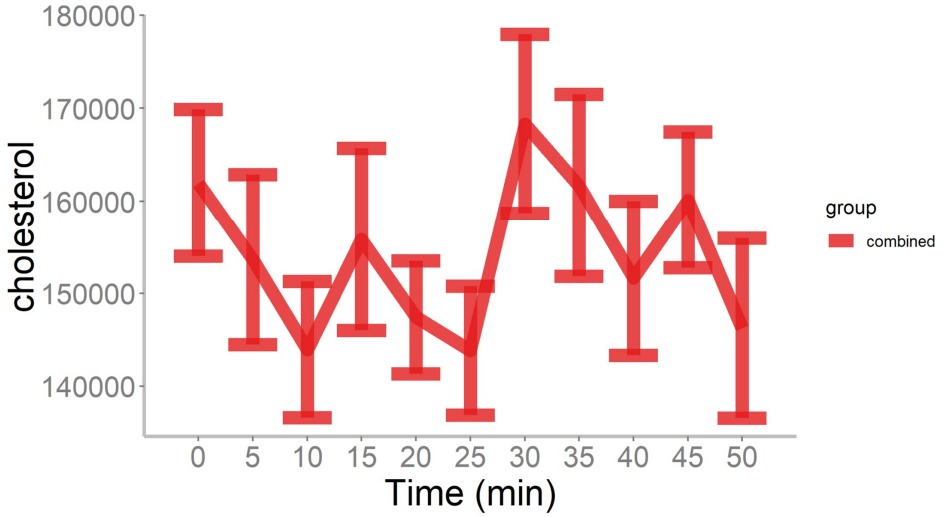

butane-2,3-diol (NIST)
4000
3000
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

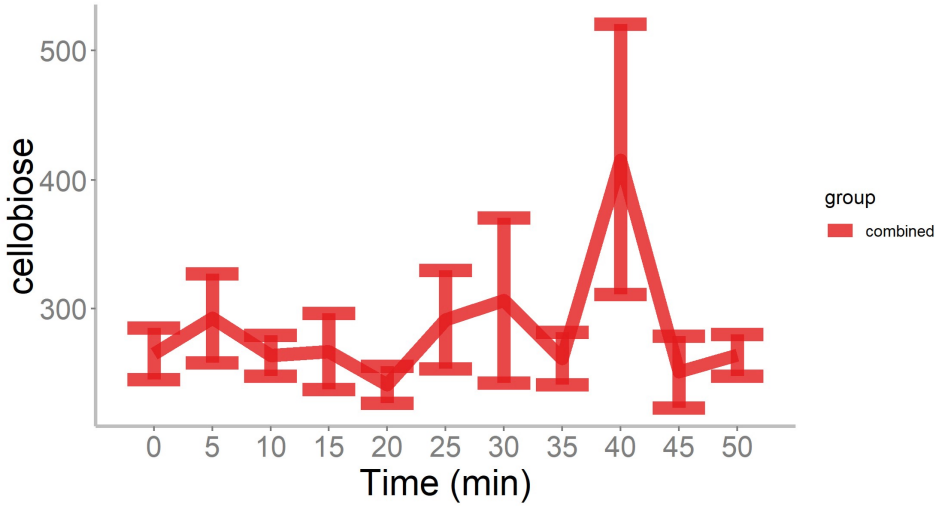

caprylic acid
1800
1700
1600
1500
1400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

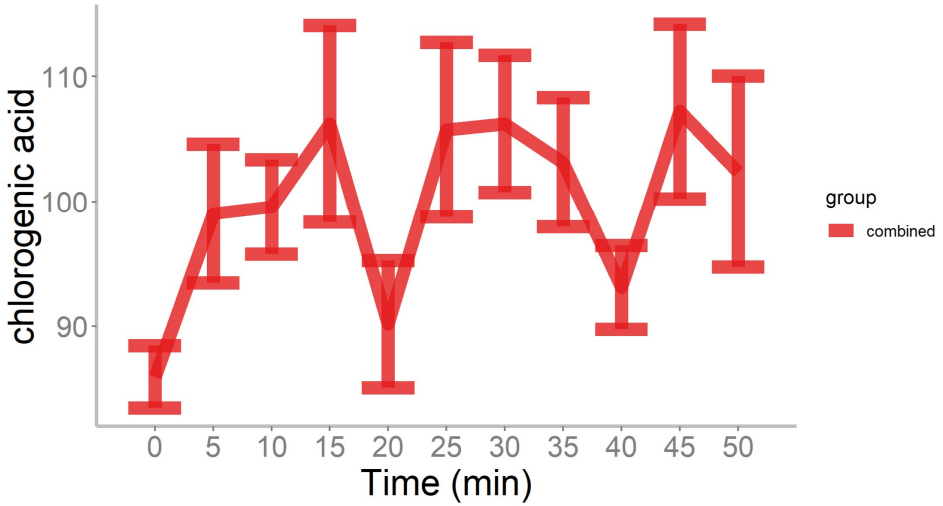

beta-alanine
550
500
450
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

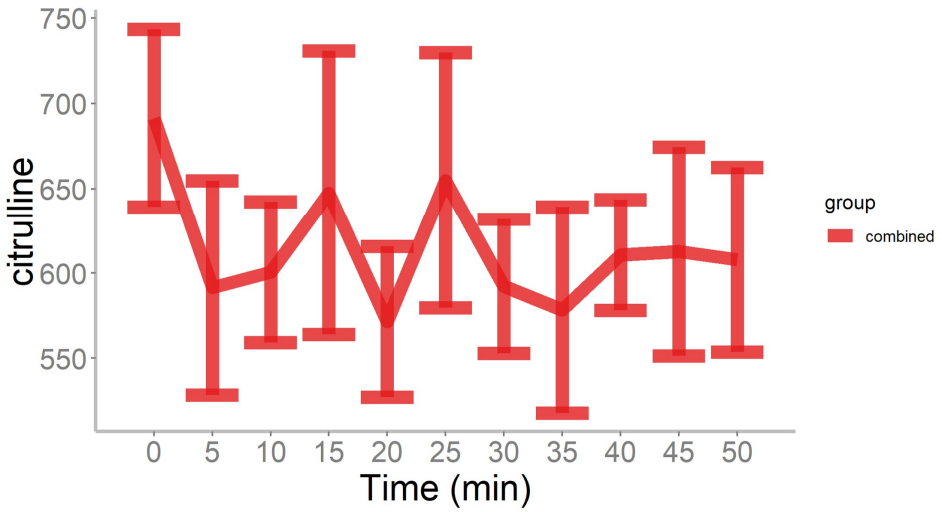

capric acid
4600
4400
4200
4000
3800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

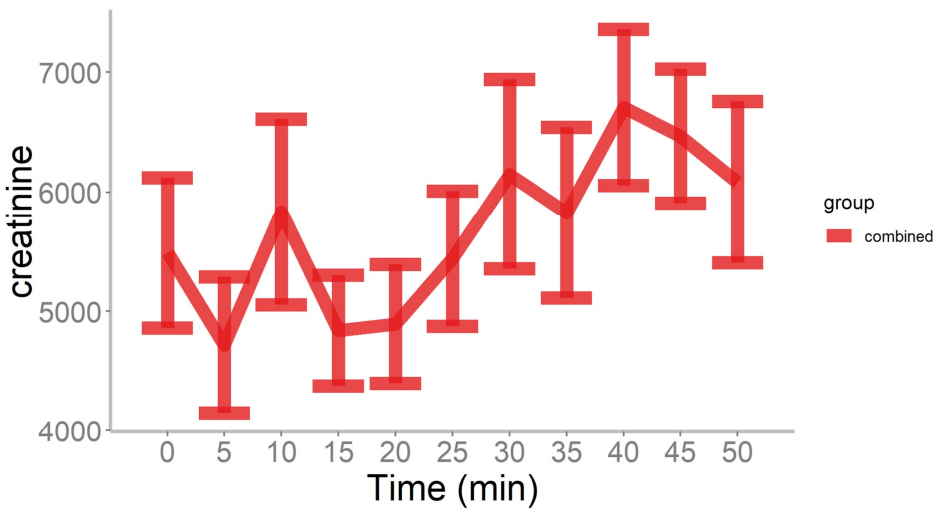

cellobiotol
200
190
180
170
160
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

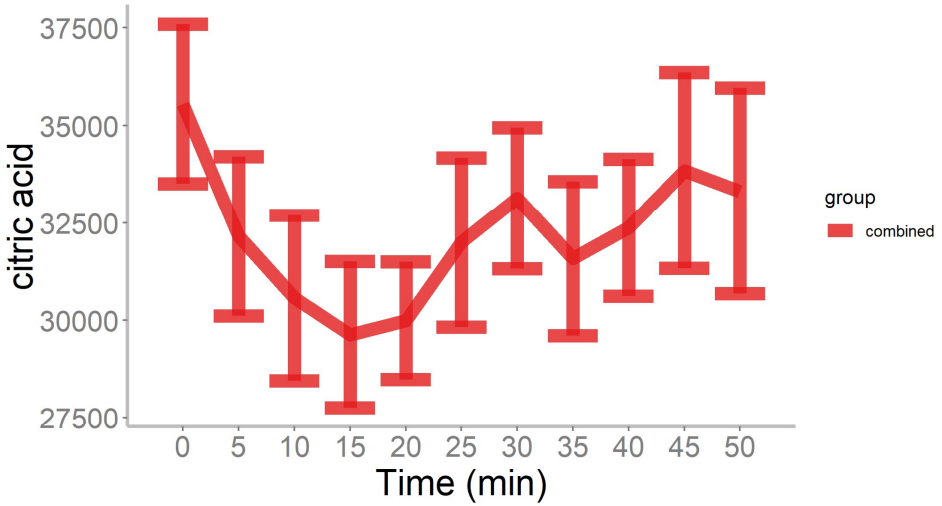

cholesterol
180000
170000
160000
150000
140000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

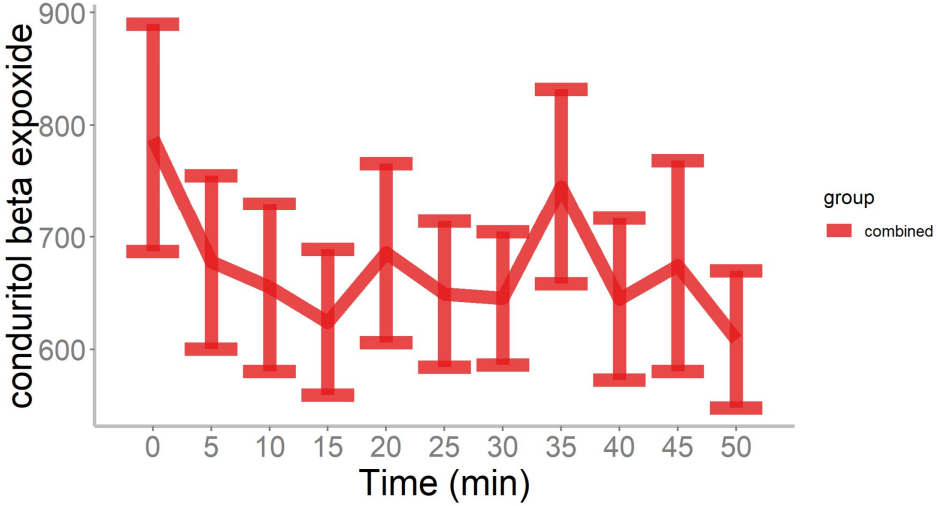

cellobiose
500
400
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

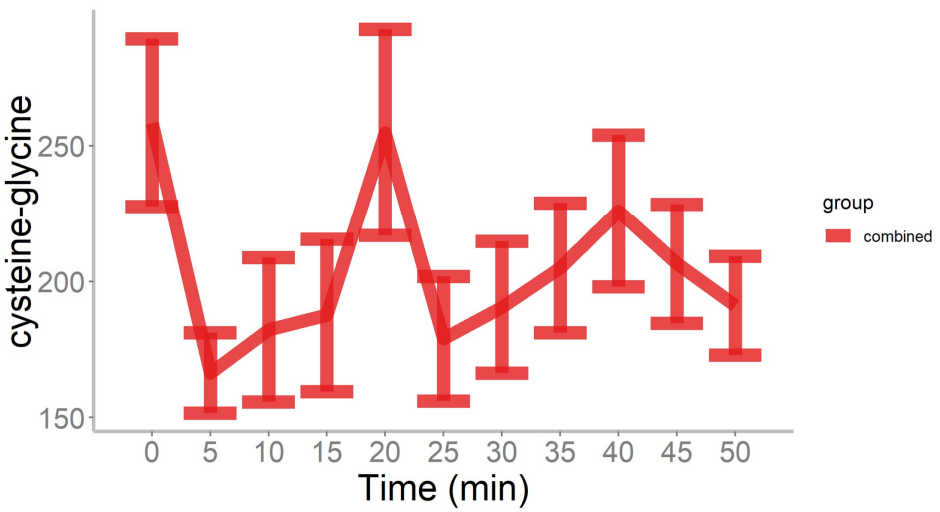

chlorogenic acid
110
100
90
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

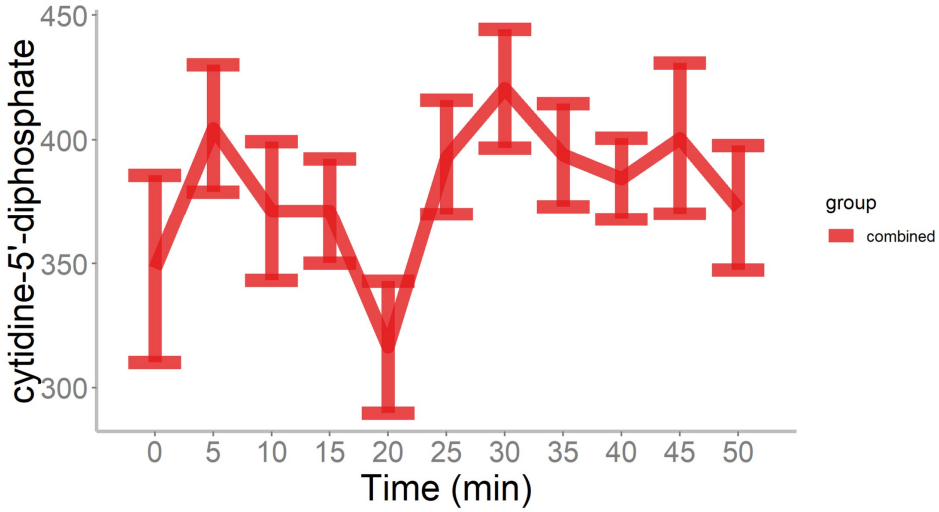

citrulline
750
700
650
600
550
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

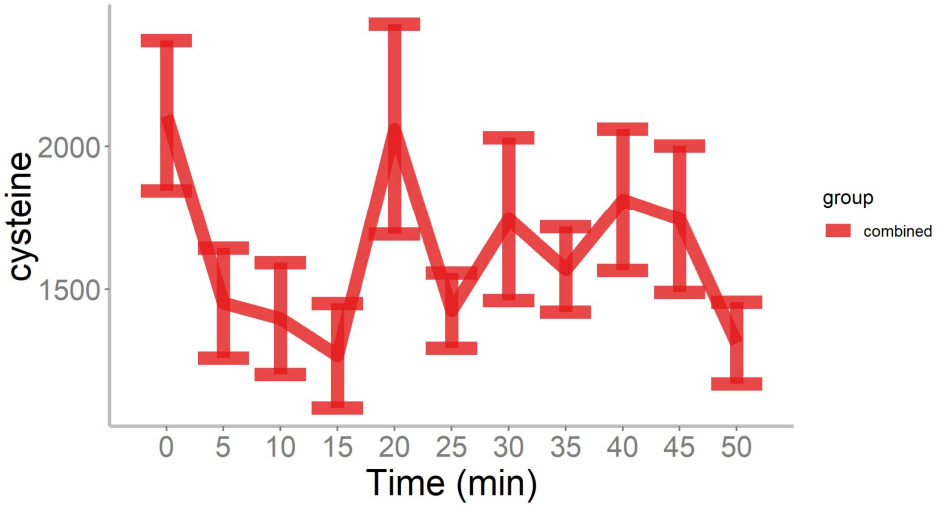

creatinine
7000
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

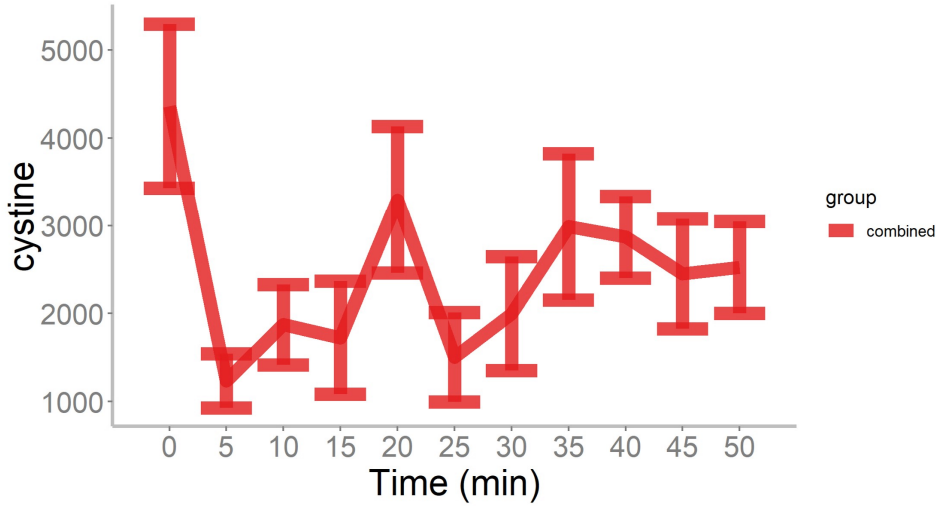

citric acid
37500
35000
32500
30000
27500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

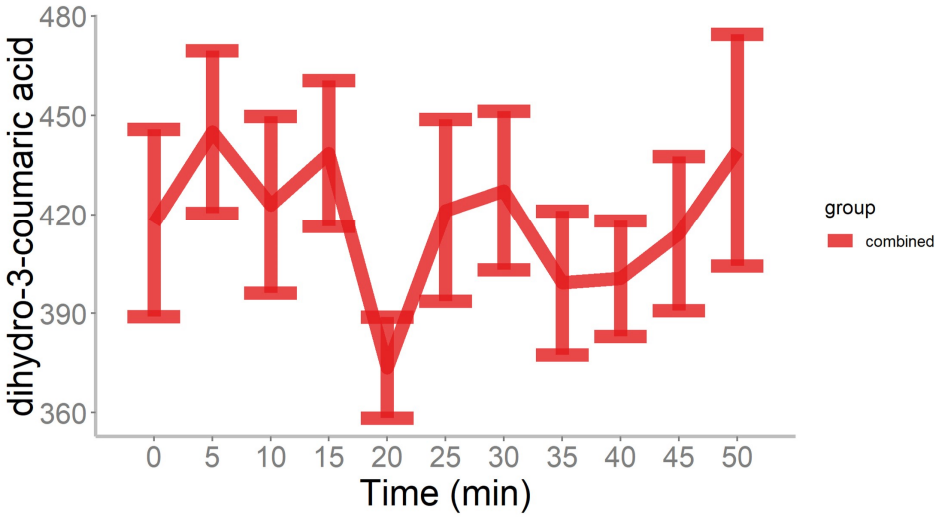

conduritol beta expoxide
900
800
700
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

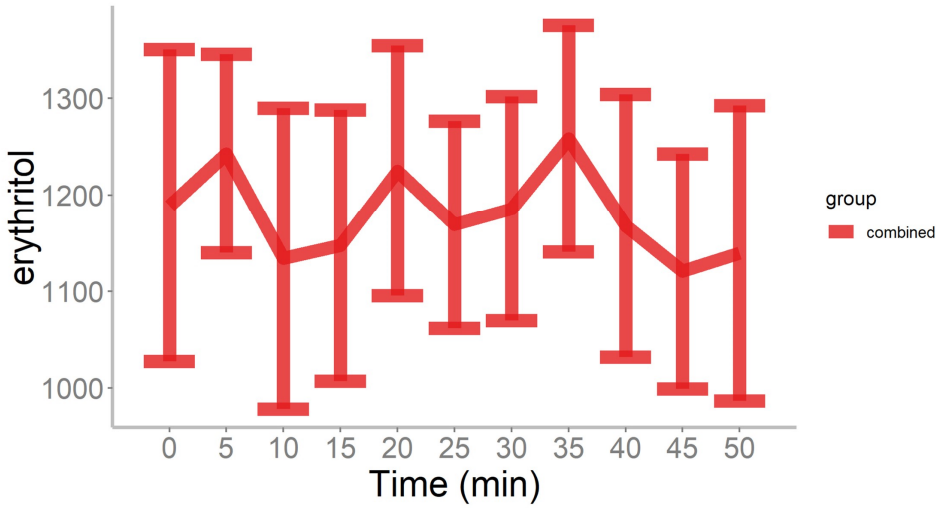

cysteine-glycine
150
200
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

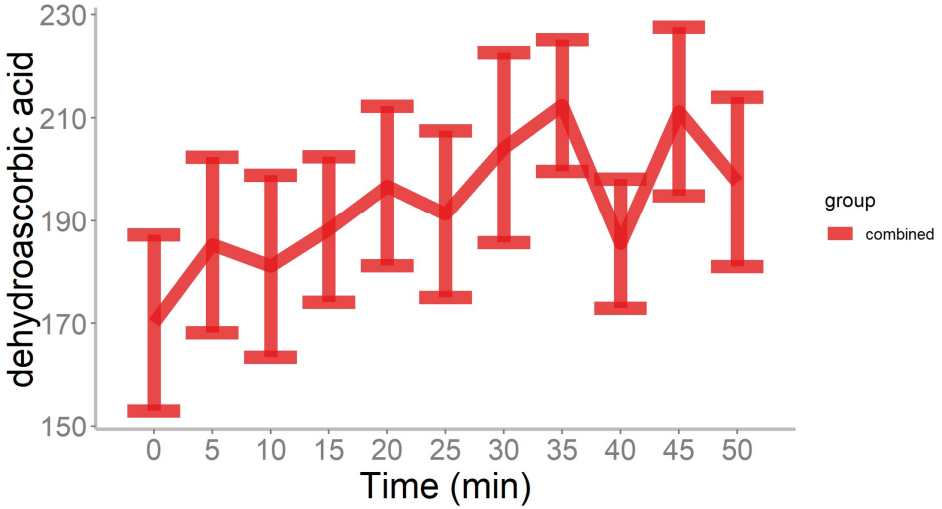

cytidine-5'-diphosphate
300
350
400
450
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

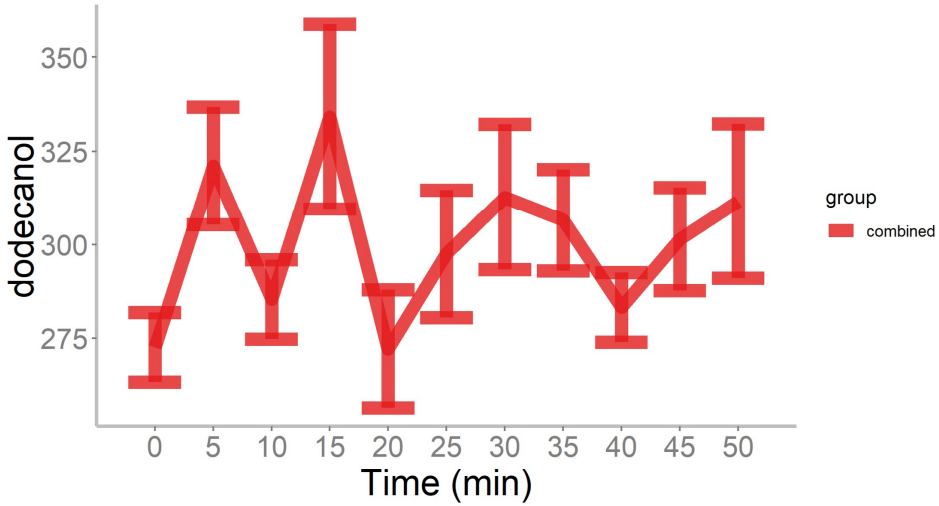

cysteine
1500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

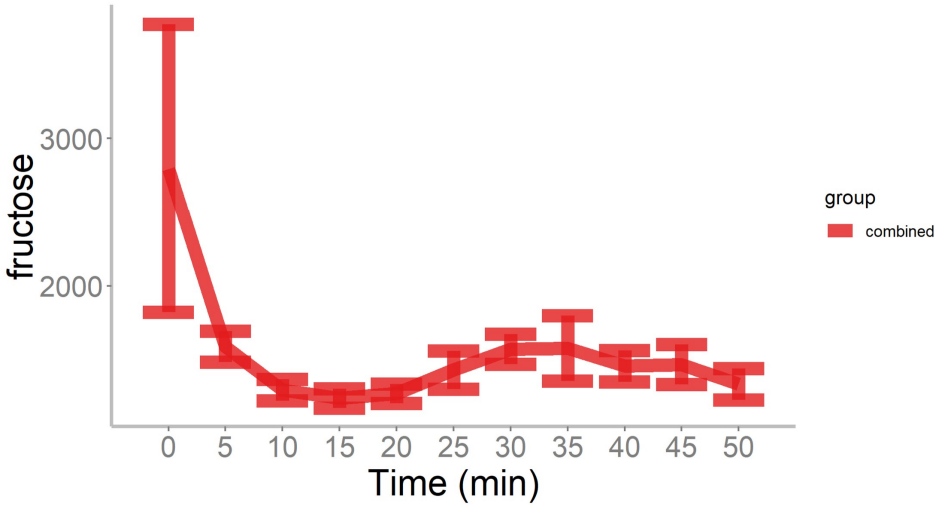

cystine
1000
2000
3000
4000
5000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

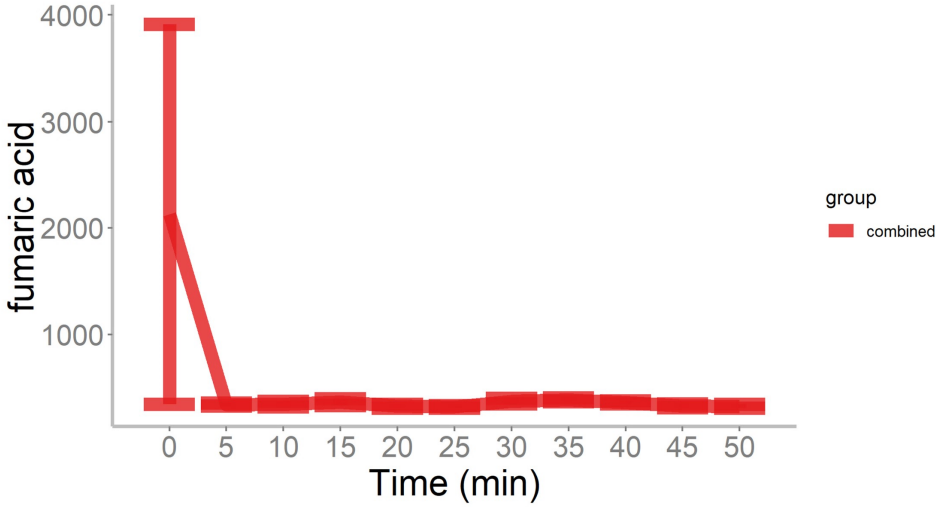

dihydro-3-coumaric acid
480
450
420
390
360
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

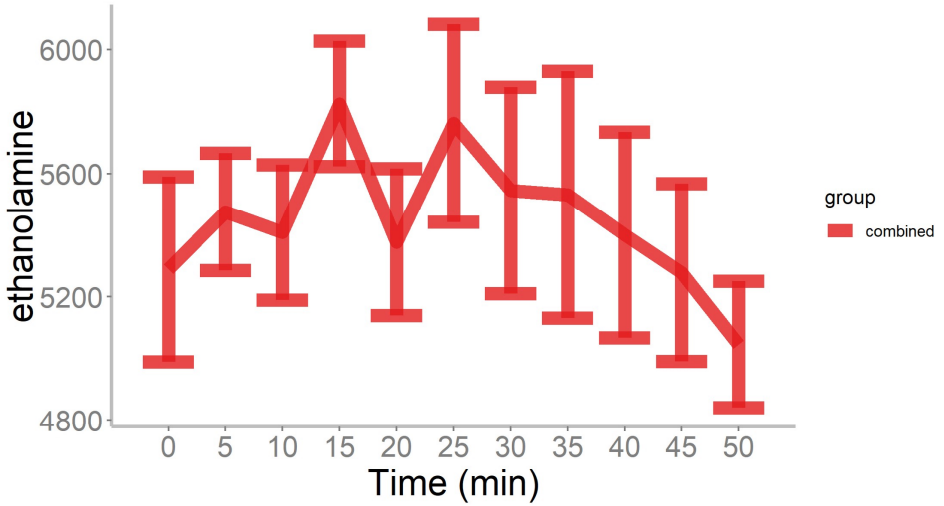

erythritol
1300
1200
1100
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

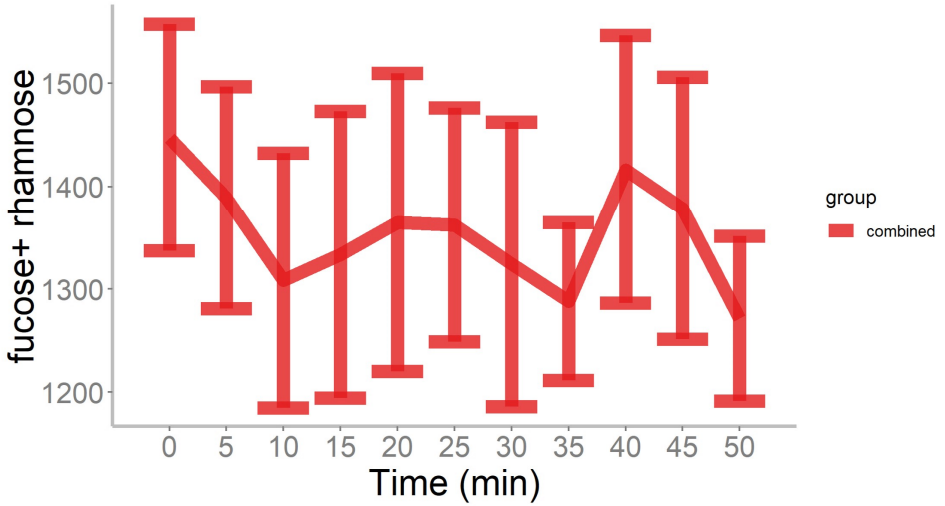

dehydroascorbic acid
230
210
190
170
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

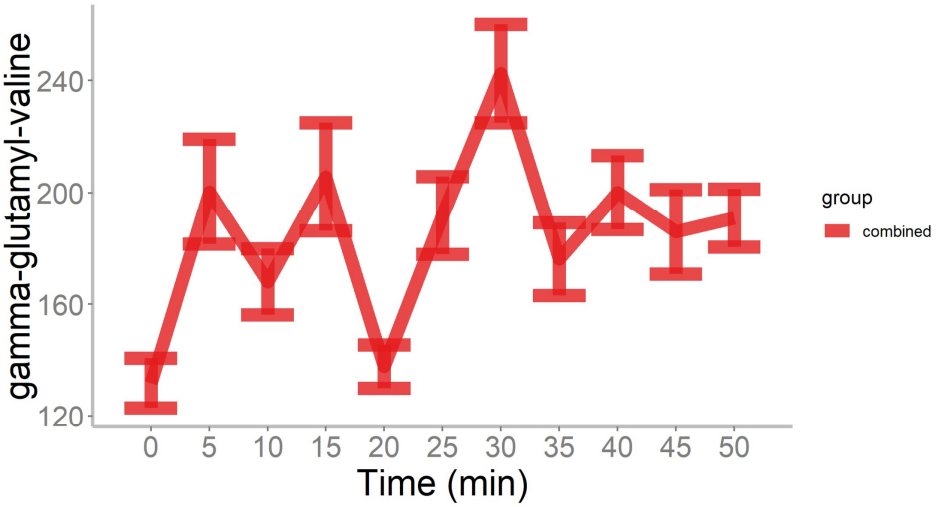

dodecanol
350
325
300
275
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

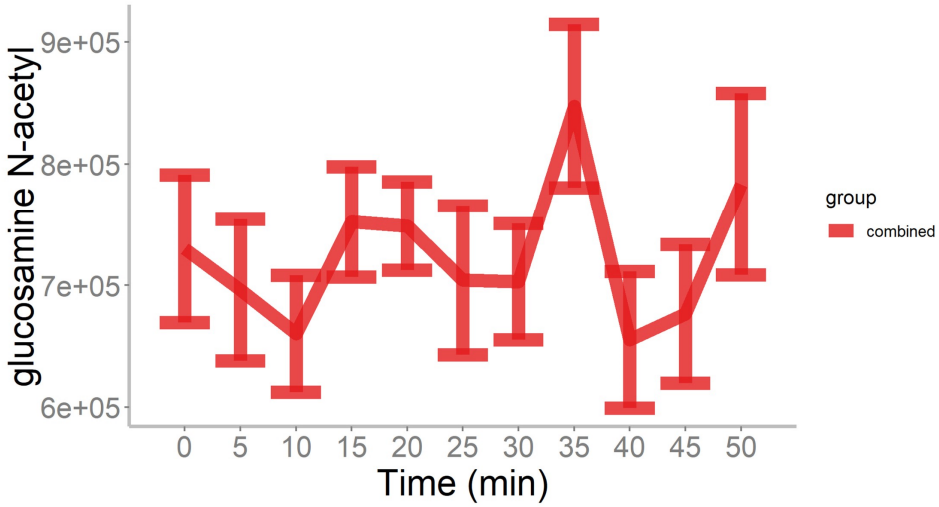

fructose
3000
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

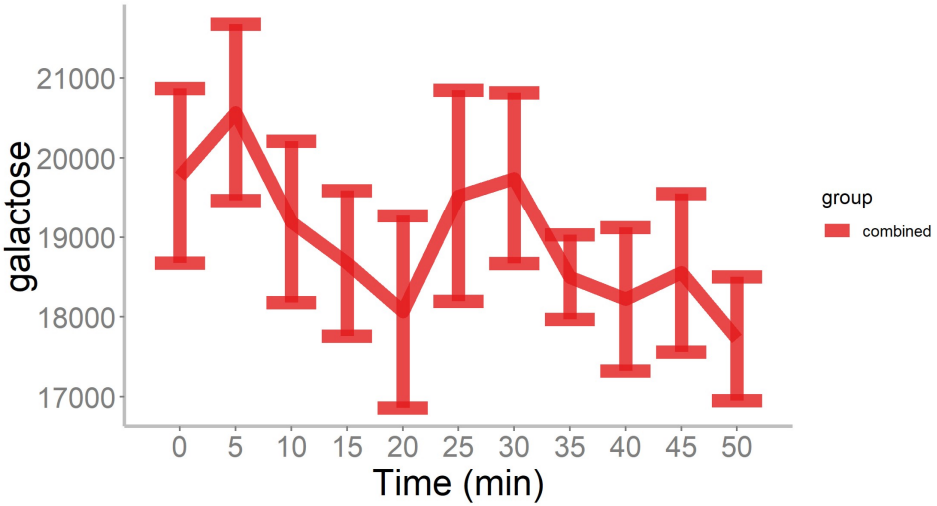

fumaric acid
4000
3000
2000
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

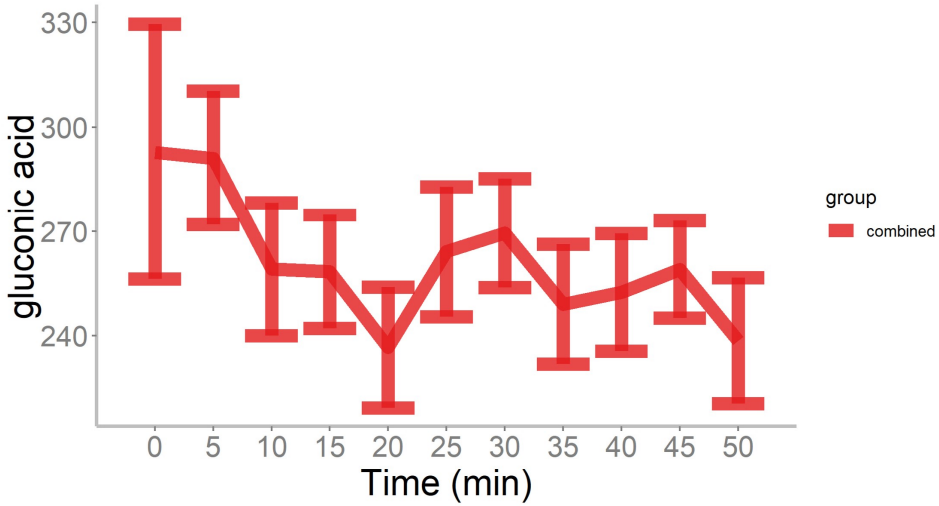

ethanolamine
6000
5600
5200
4800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

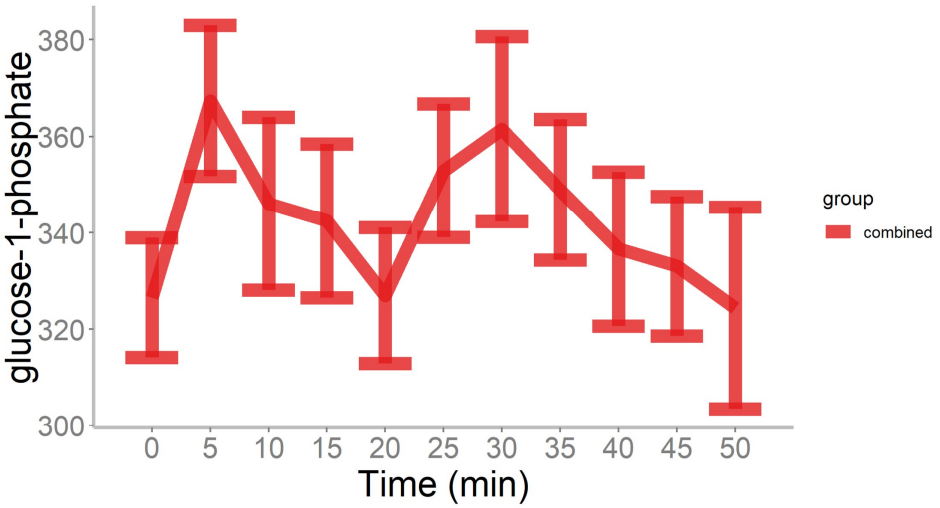

fucose+ rhamnose
1500
1400
1300
1200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

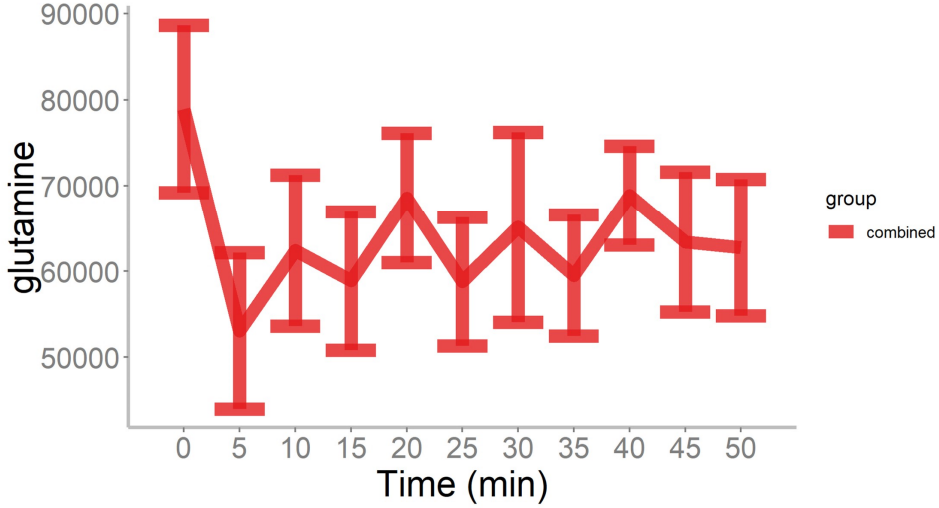

gamma-glutamyl-valine
240
200
160
120
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

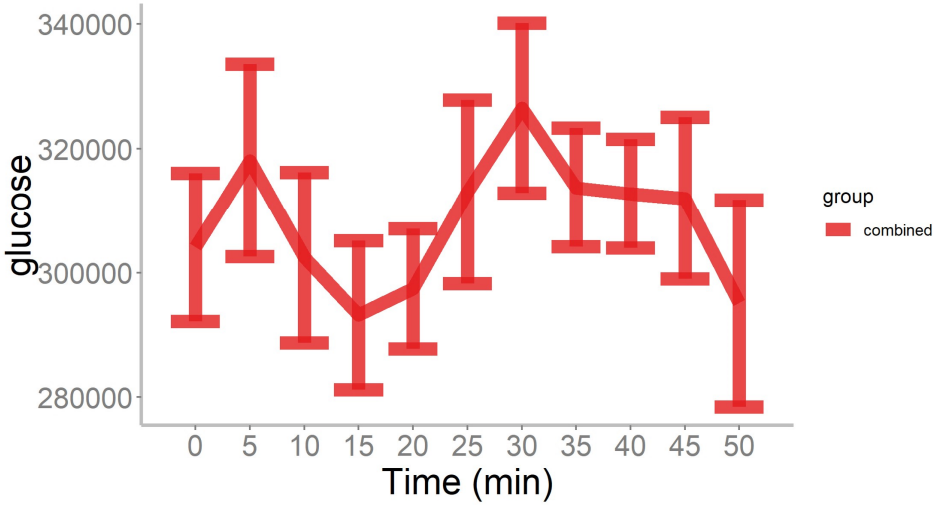

glucosamine N-acetyl
9e+05
8e+05
7e+05
6e+05
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

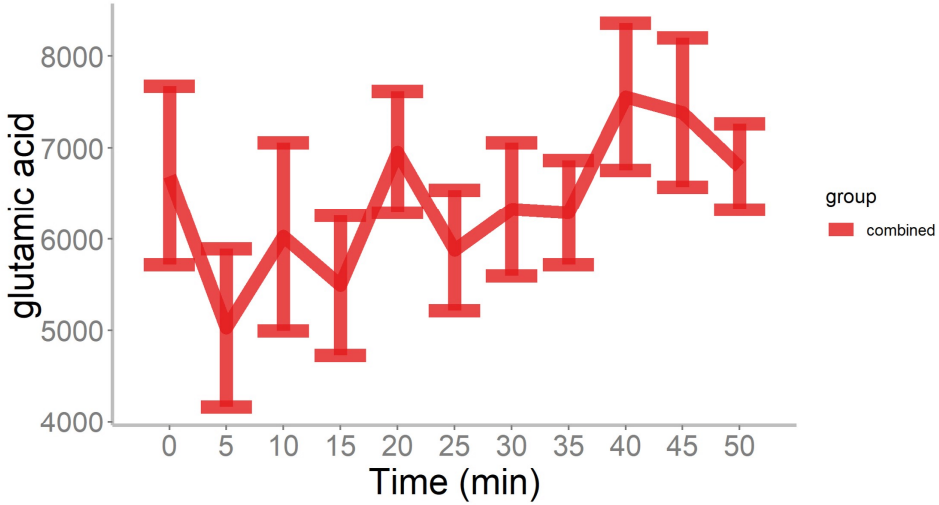

galactose
21000
20000
19000
18000
17000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


gluconic acid
330
300
270
240
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glucose-1-phosphate
380
360
340
320
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glutamine
90000
80000
70000
60000
50000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glucose
340000
320000
300000
280000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glutamic acid
8000
7000
6000
5000
4000
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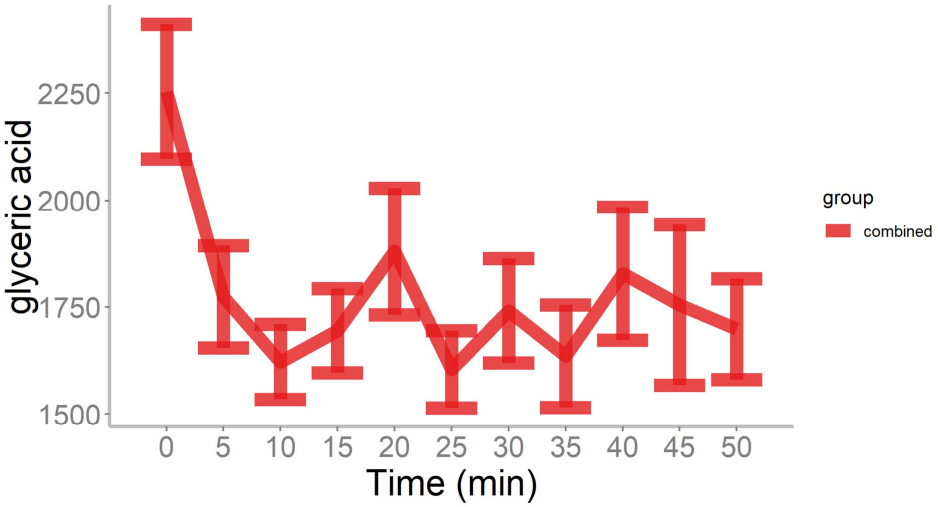
Time (min)
group
combined


glyceric acid
2250
2000
1750
1500
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Time (min)
group
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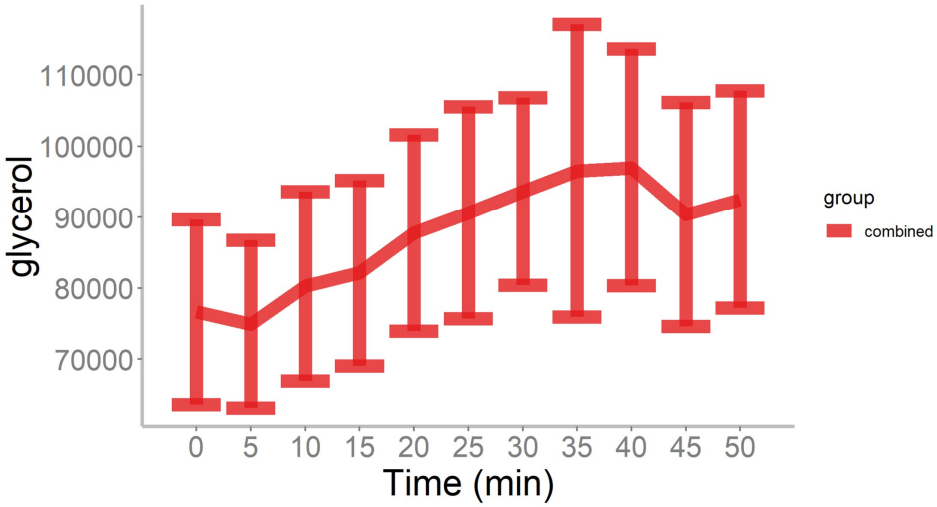
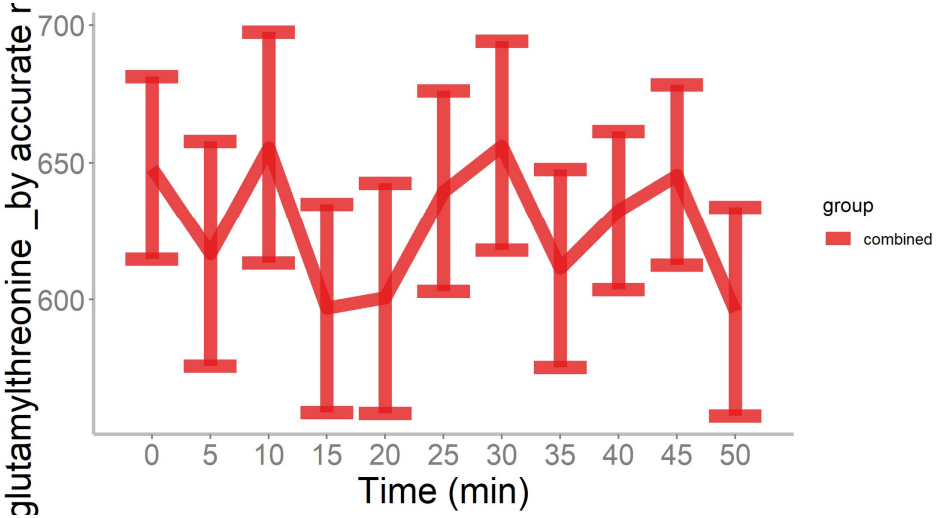
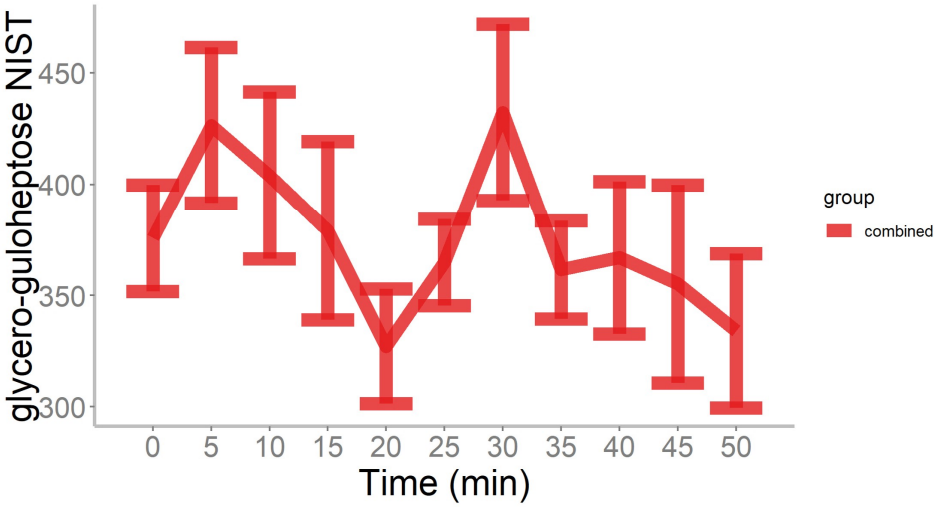
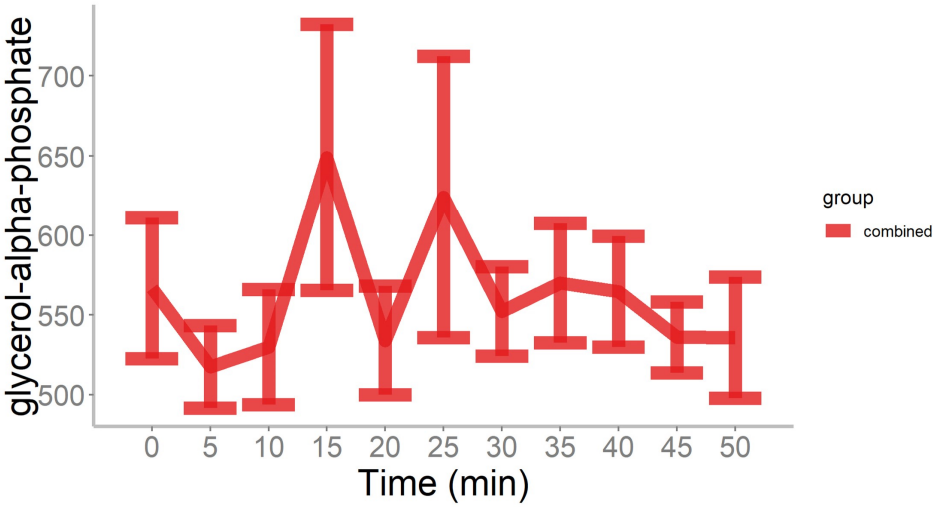

glycerol
110000
100000
90000
80000
70000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glutamylthreonine _by accurate r
700
650
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glycero-guloheptose NIST
450
400
350
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


glycerol-alpha-phosphate
700
650
600
550
500
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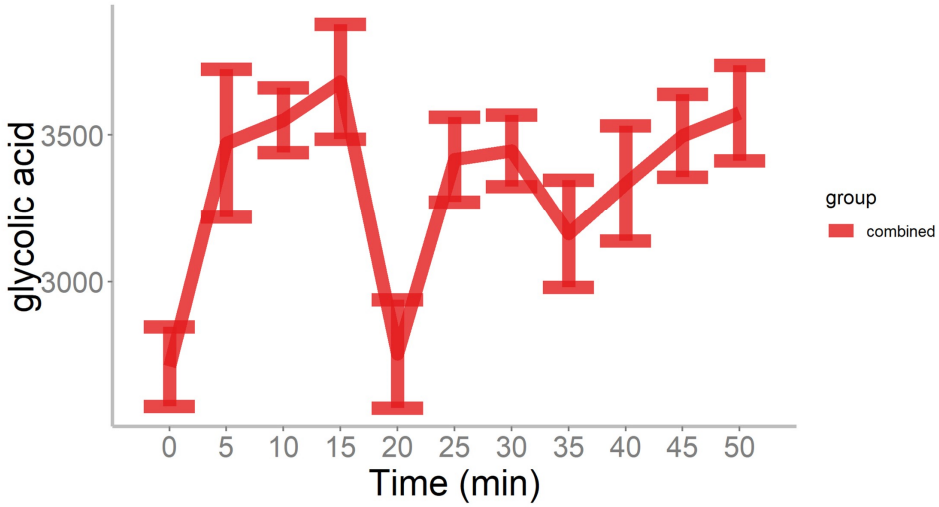
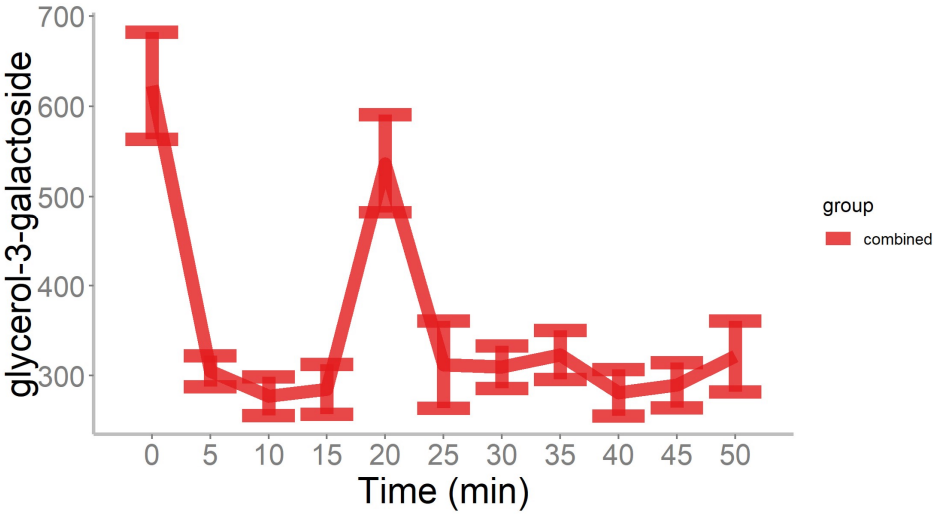
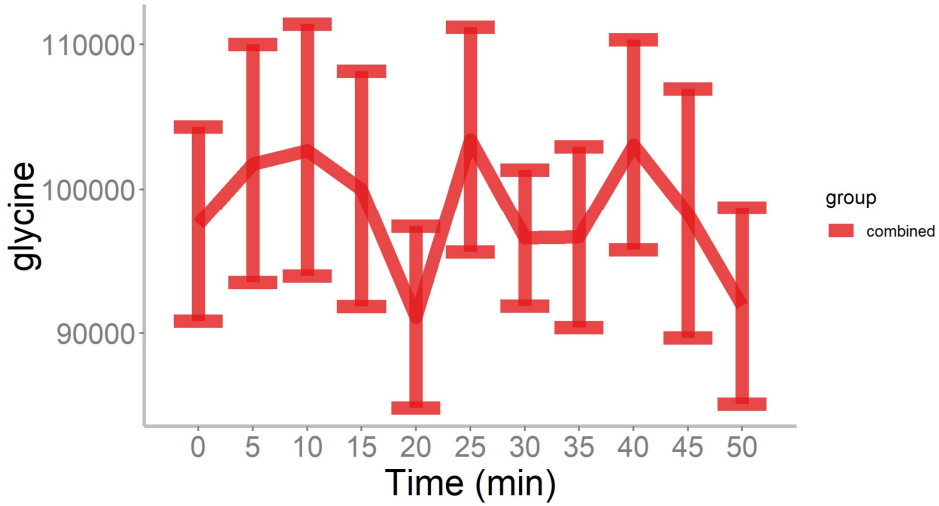
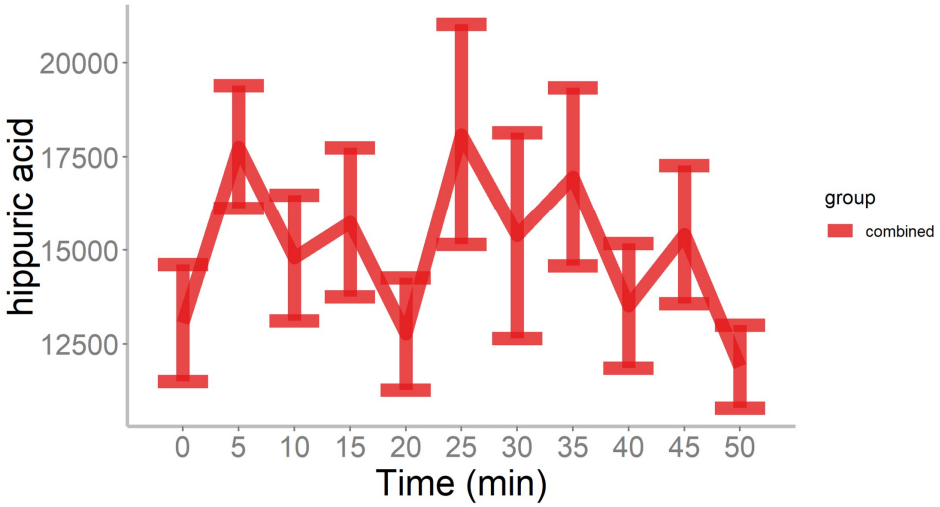
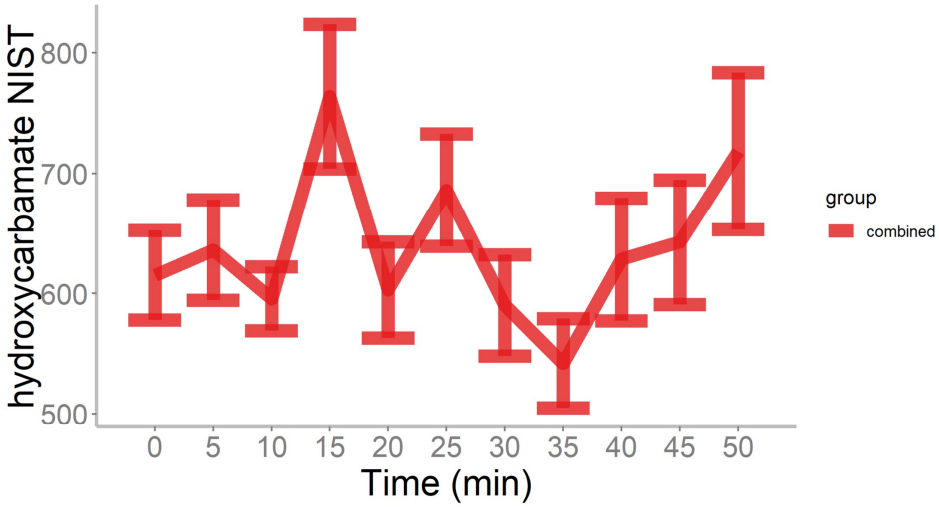
Time (min)
group
combined

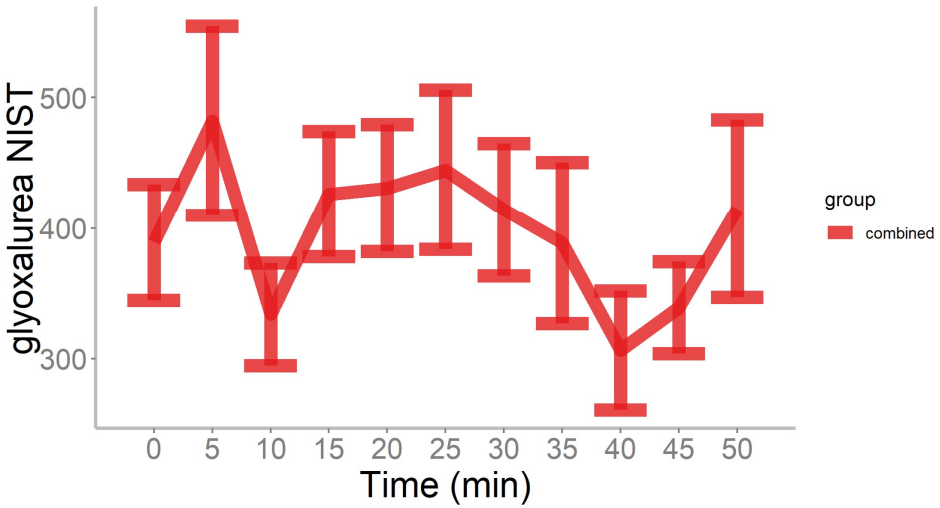

glycolic acid
3500
3000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

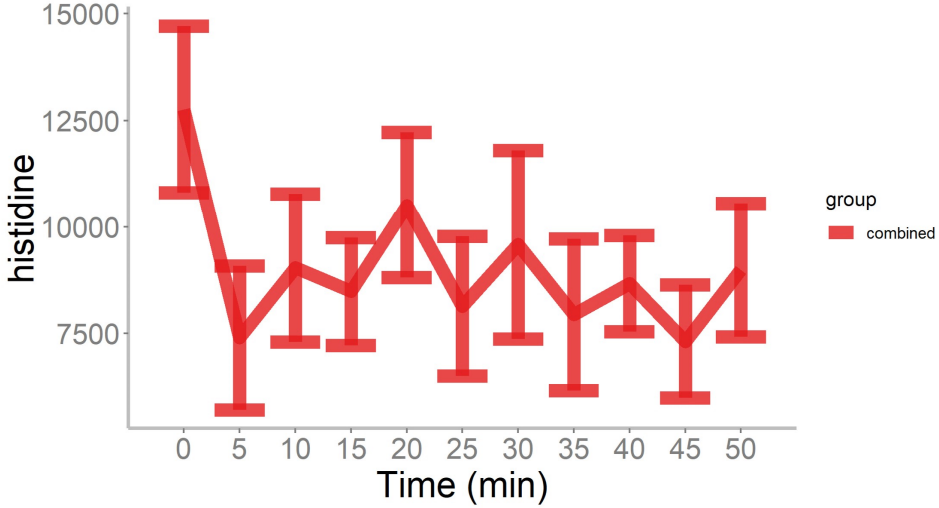

glycerol-3-galactoside
700
600
500
400
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

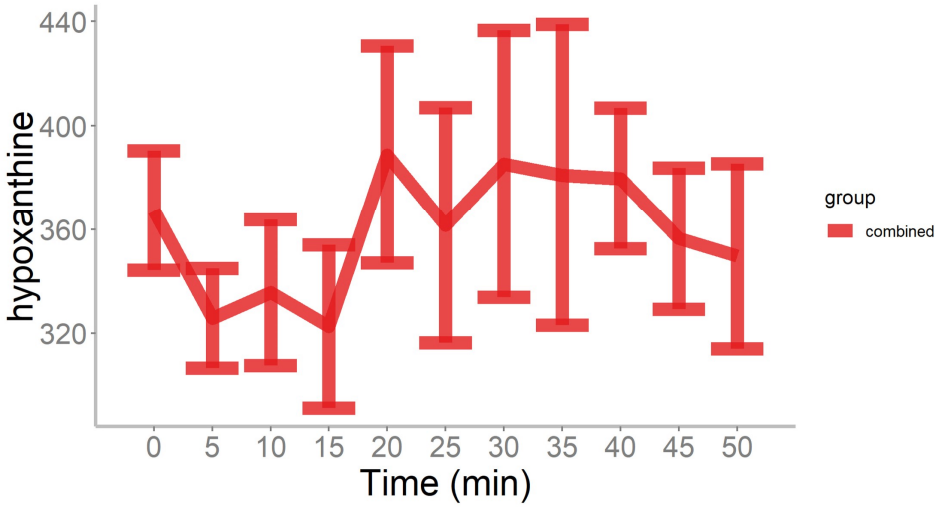

glycine
110000
100000
90000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

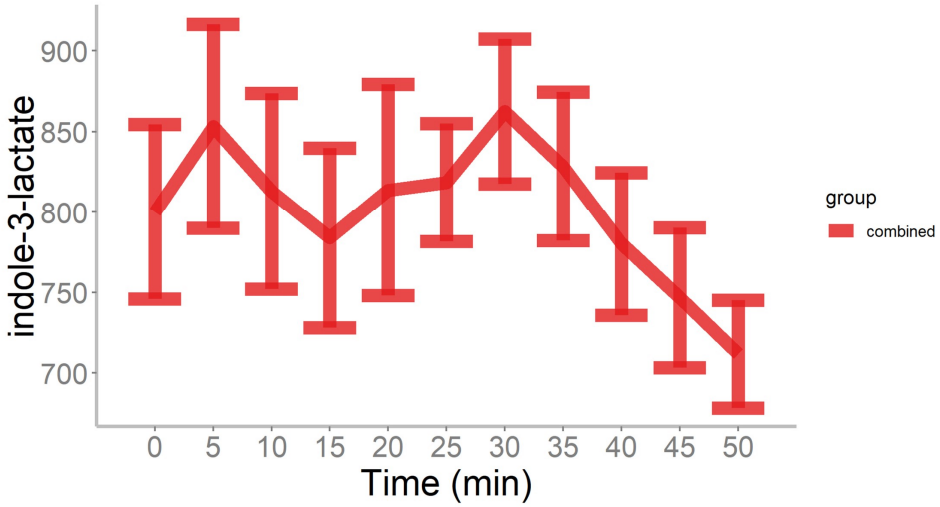

hippuric acid
20000
17500
15000
12500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

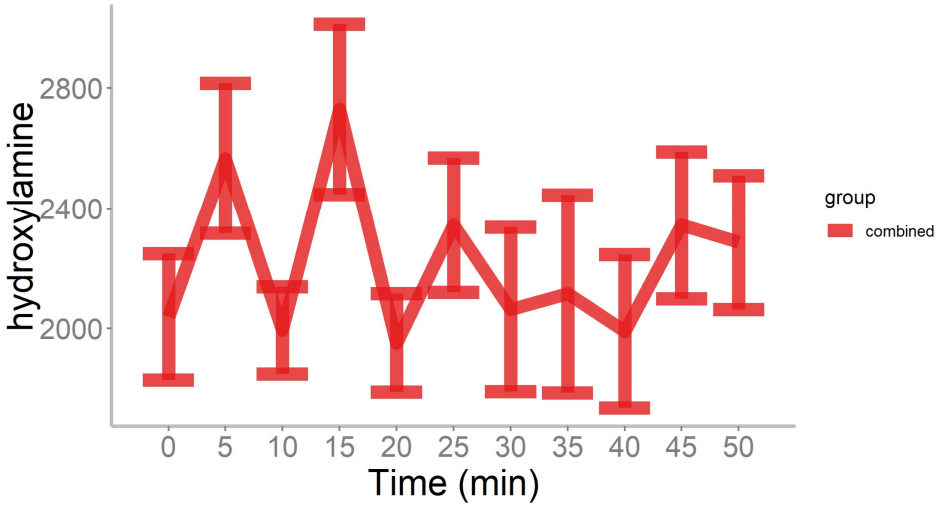

hydroxycarbamate NIST
800
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

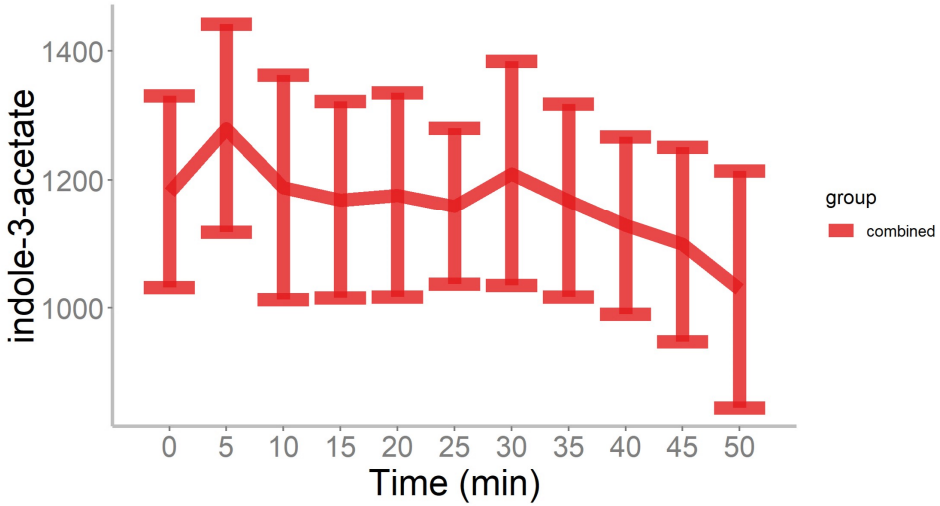

glyoxalurea NIST
500
400
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

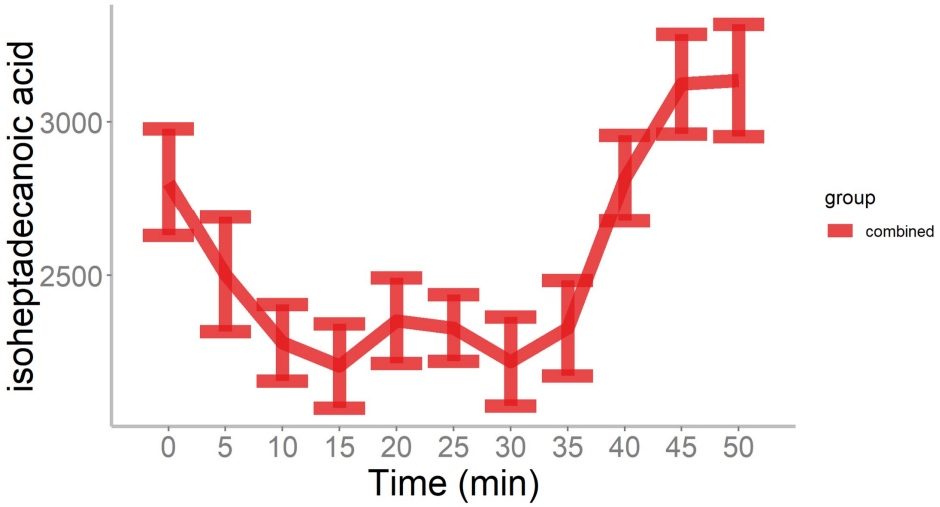

histidine
15000
12500
10000
7500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

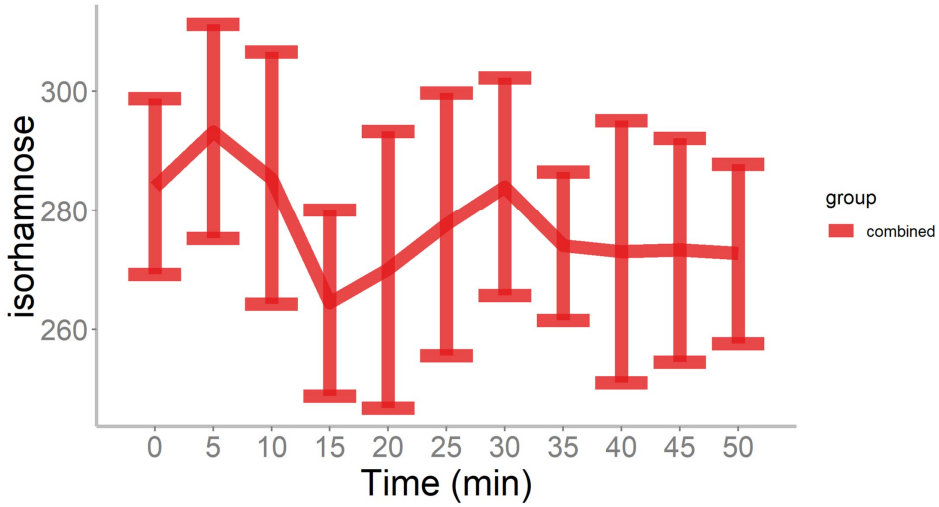

hypoxanthine
440
400
360
320
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

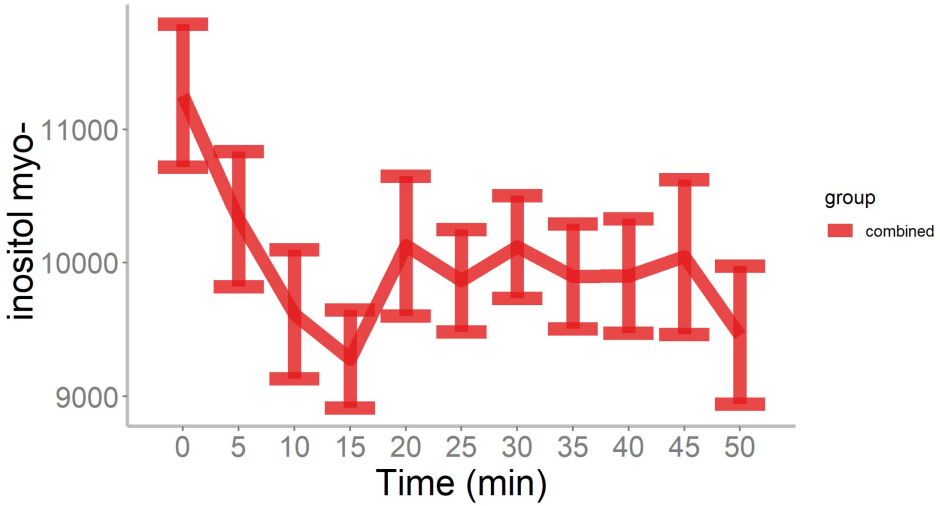

indole-3-lactate
900
850
800
750
700
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

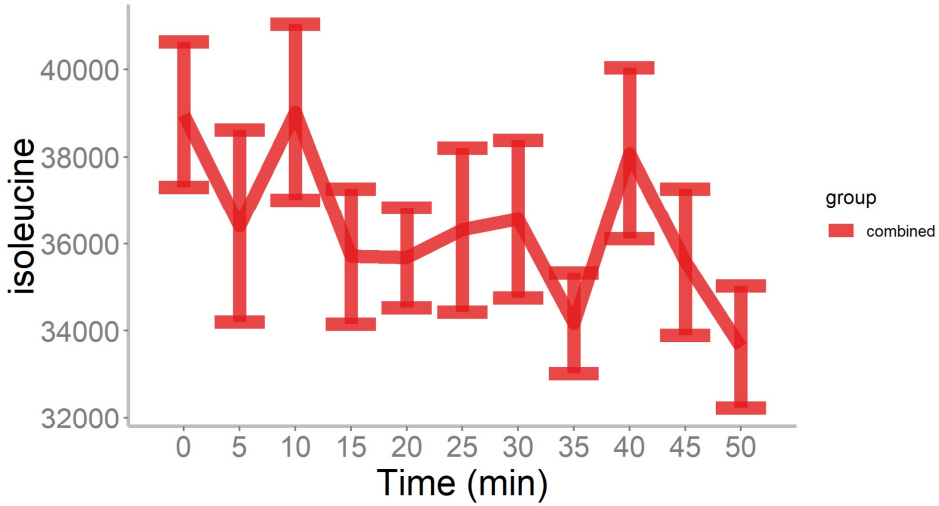

hydroxylamine
2800
2400
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

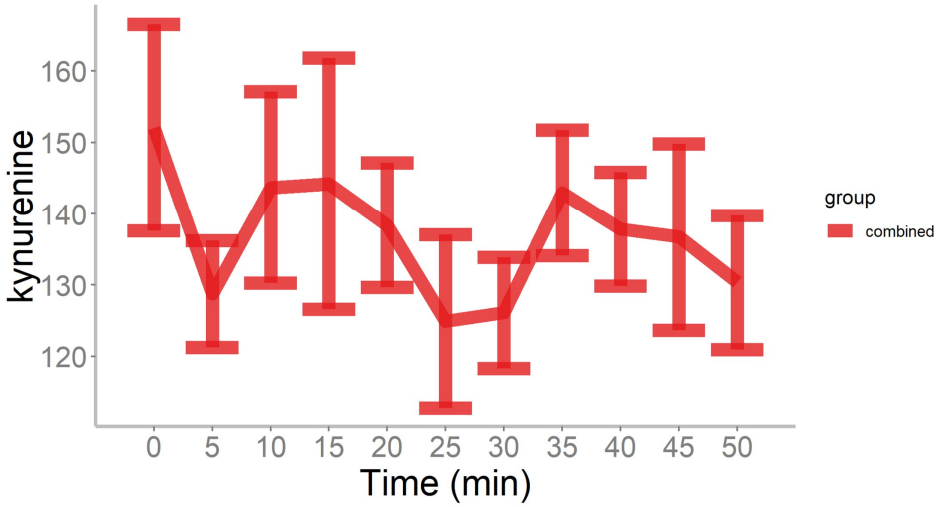

indole-3-acetate
1400
1200
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

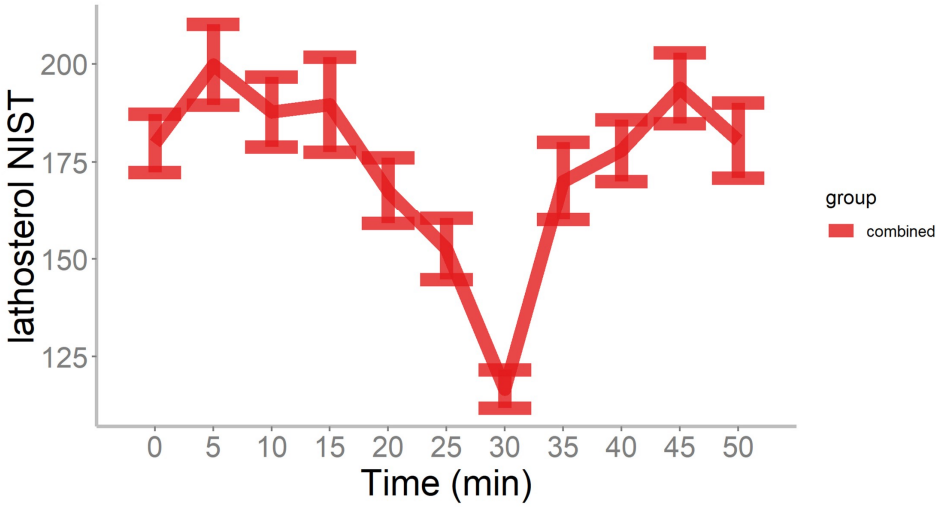

isoheptadecanoic acid
3000
2500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

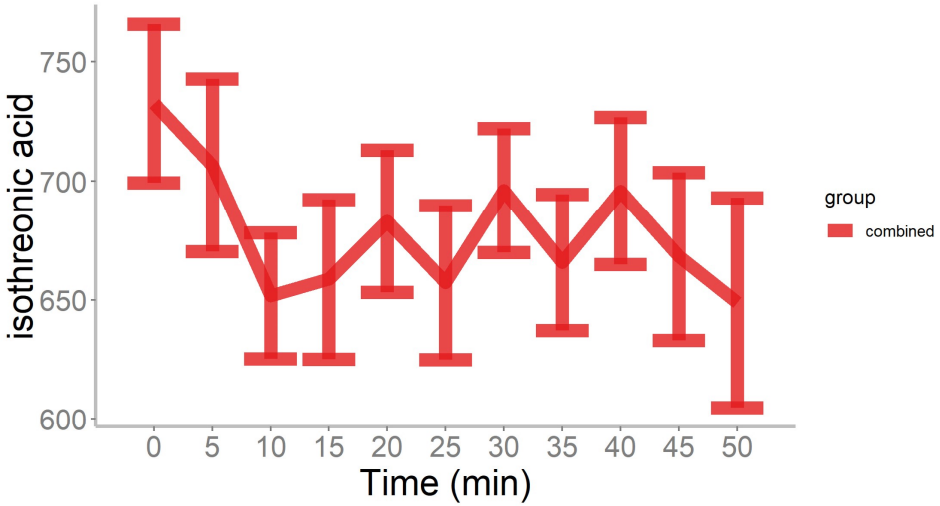

isorhamnose
300
280
260
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

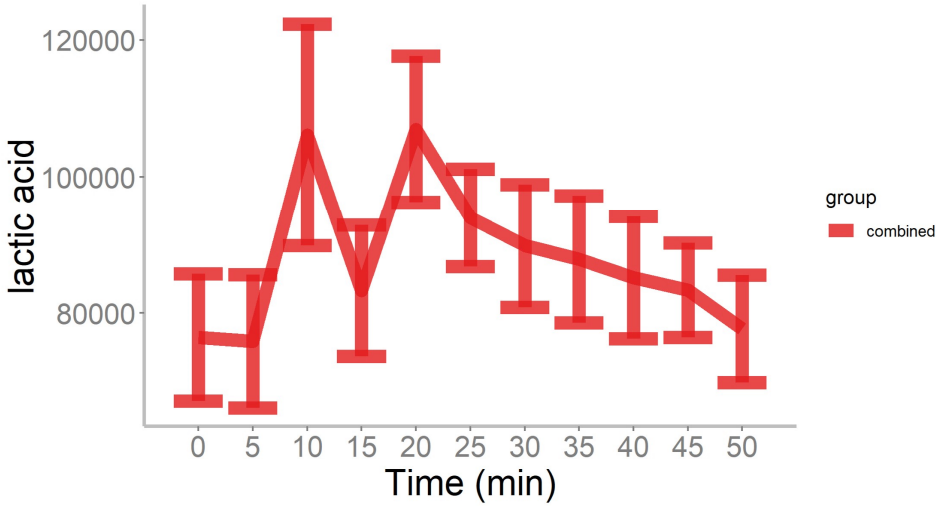

inositol myo-
11000
10000
9000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

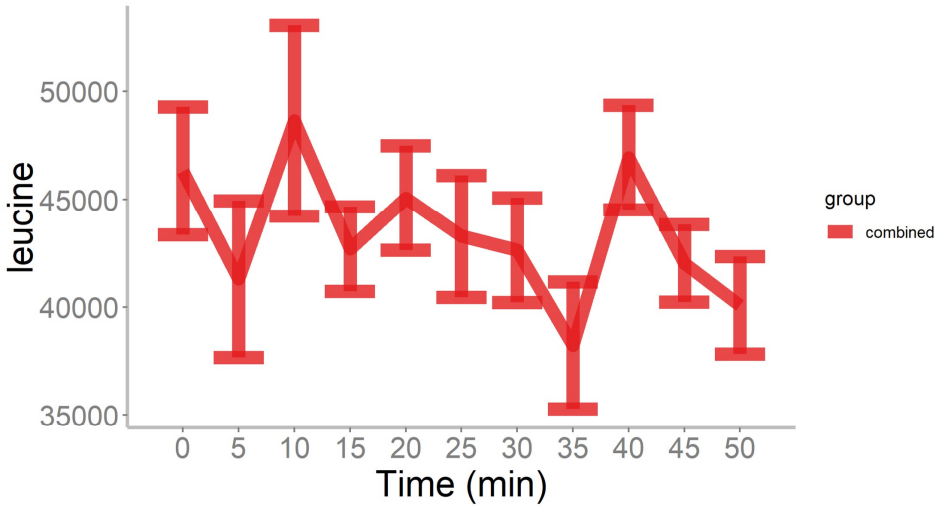

isoleucine
40000
38000
36000
34000
32000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

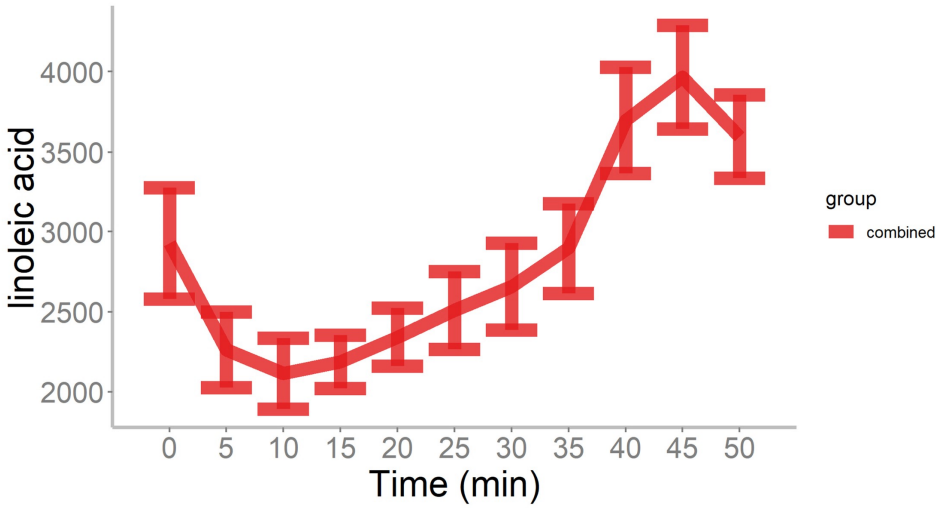

kynurenine
160
150
140
130
120
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

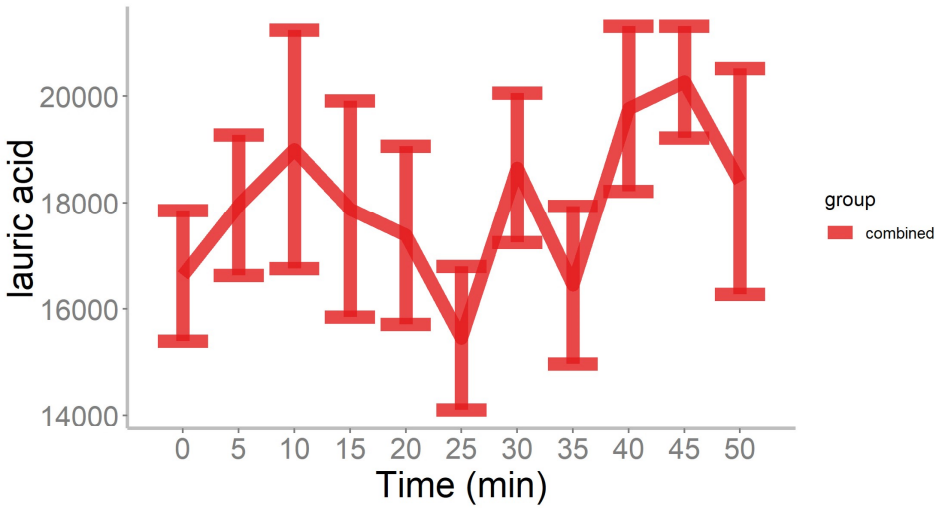

lathosterol NIST
200
175
150
125
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

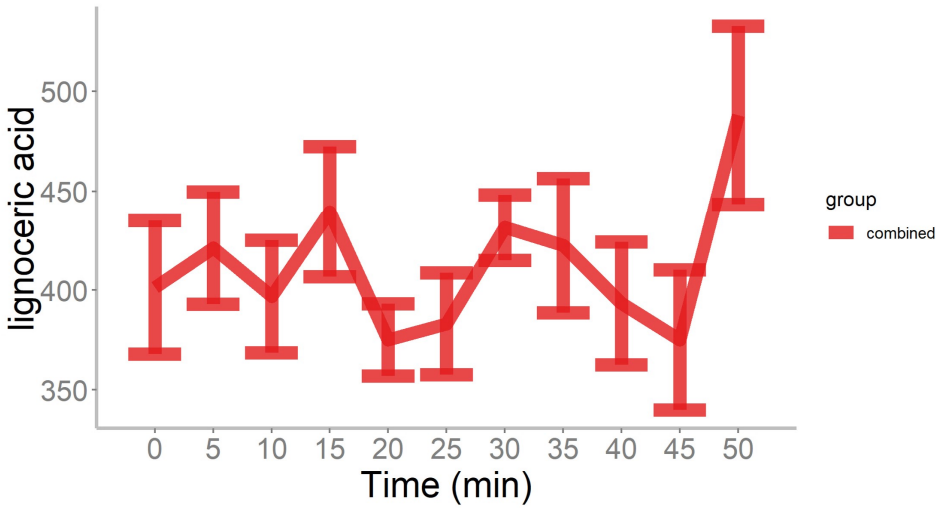

isothreonic acid
750
700
650
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

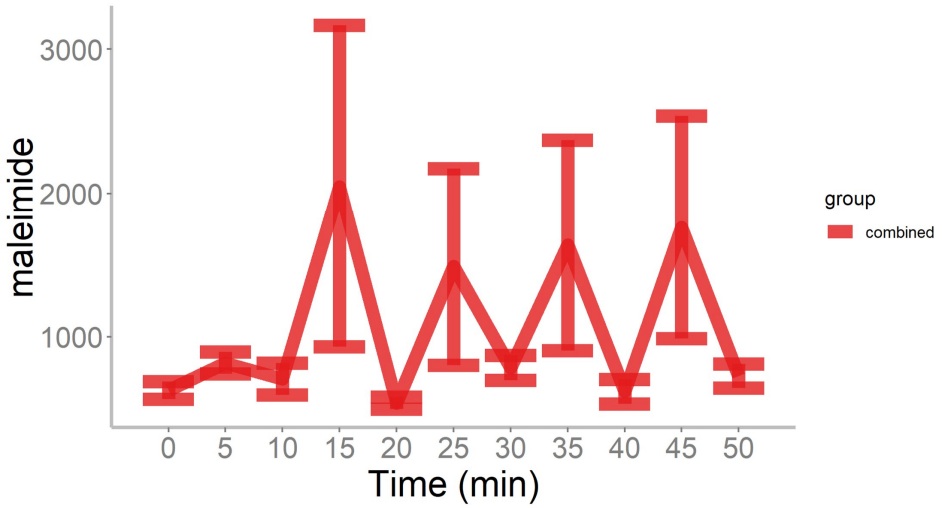

lactic acid
120000
100000
80000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

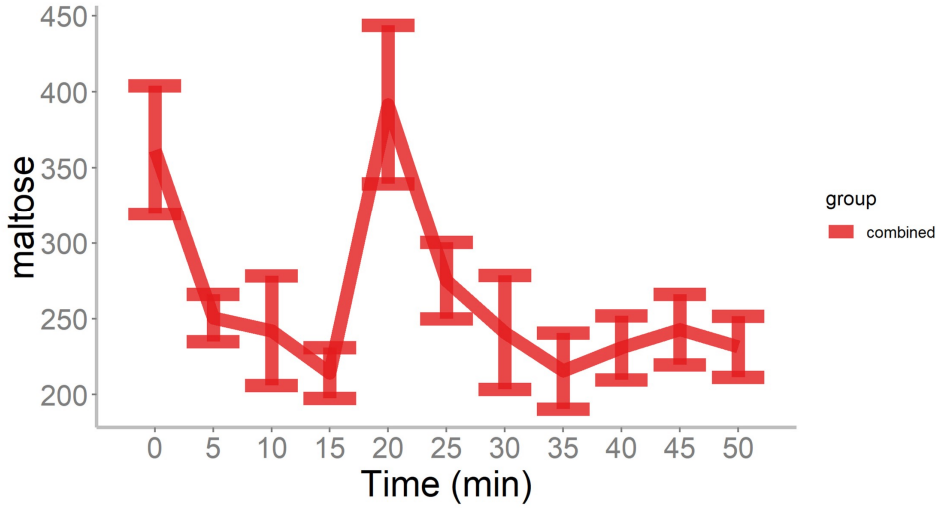

leucine
50000
45000
40000
35000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

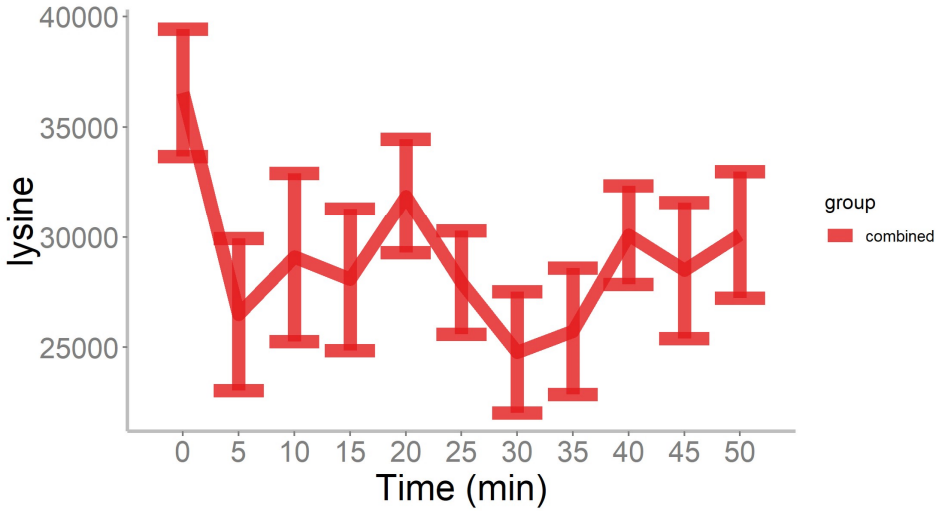

linoleic acid
4000
3500
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

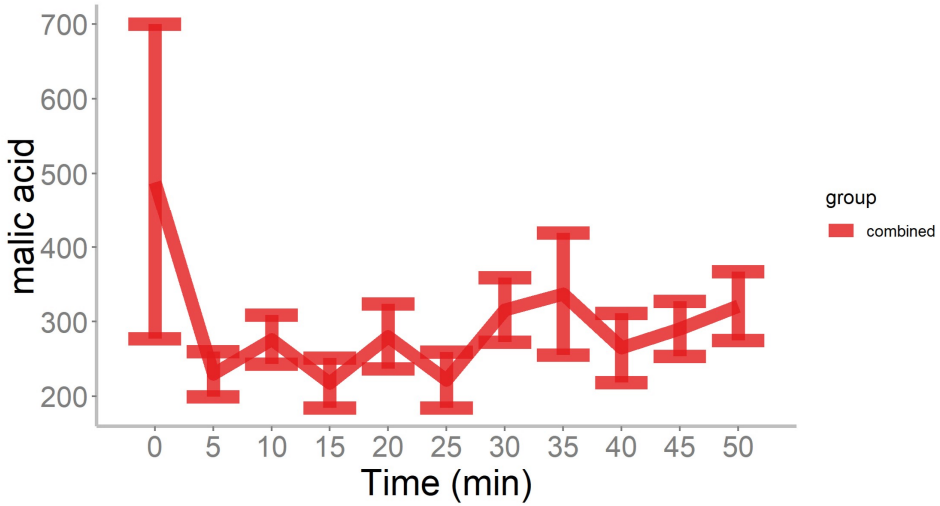

lauric acid
20000
18000
16000
14000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

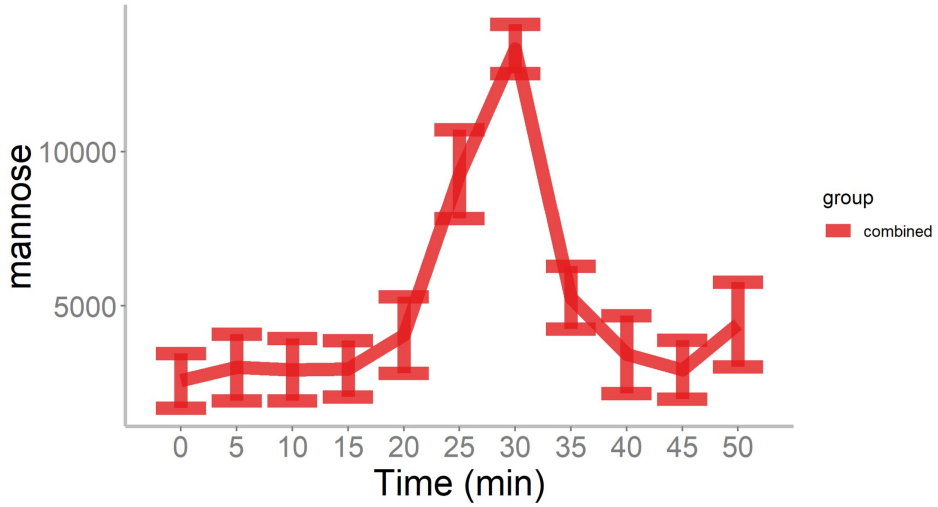

lignoceric acid
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

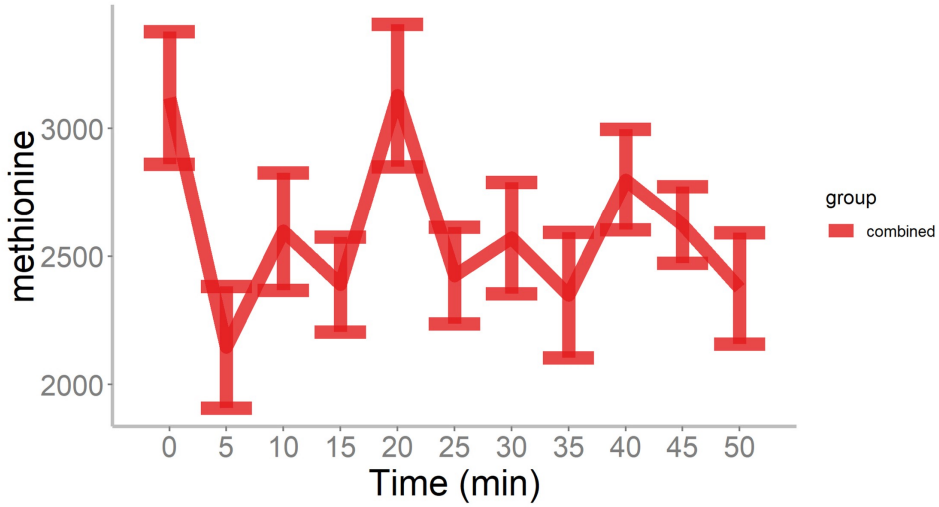

maleimide
3000
2000
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

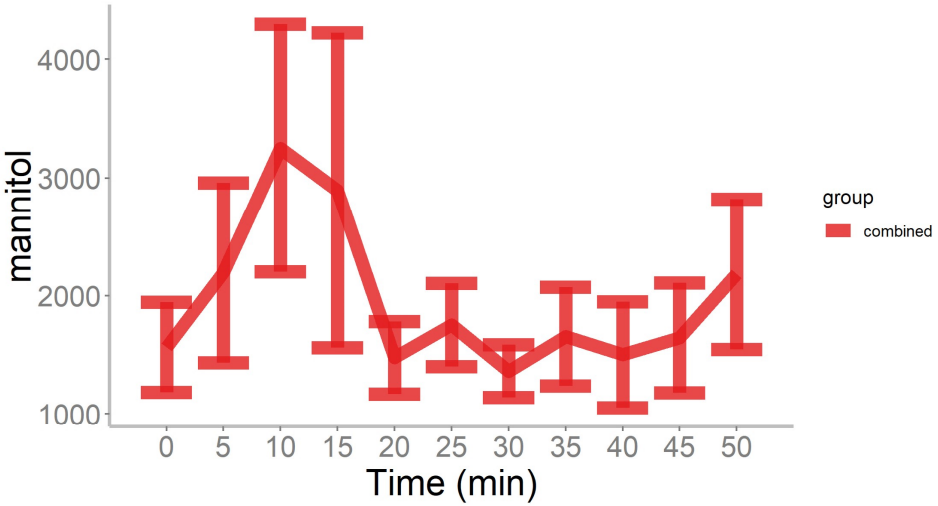

maltose
450
400
350
300
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

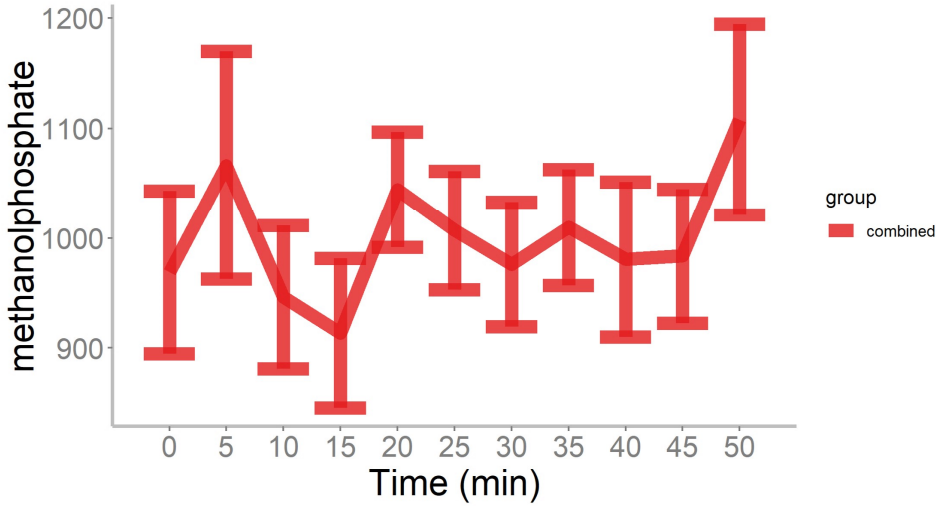

lysine
40000
35000
30000
25000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

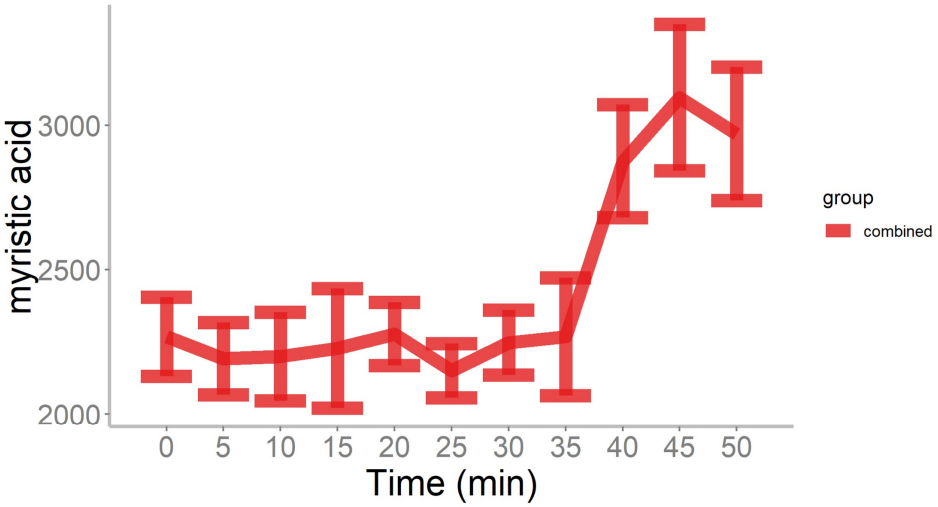

malic acid
700
600
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

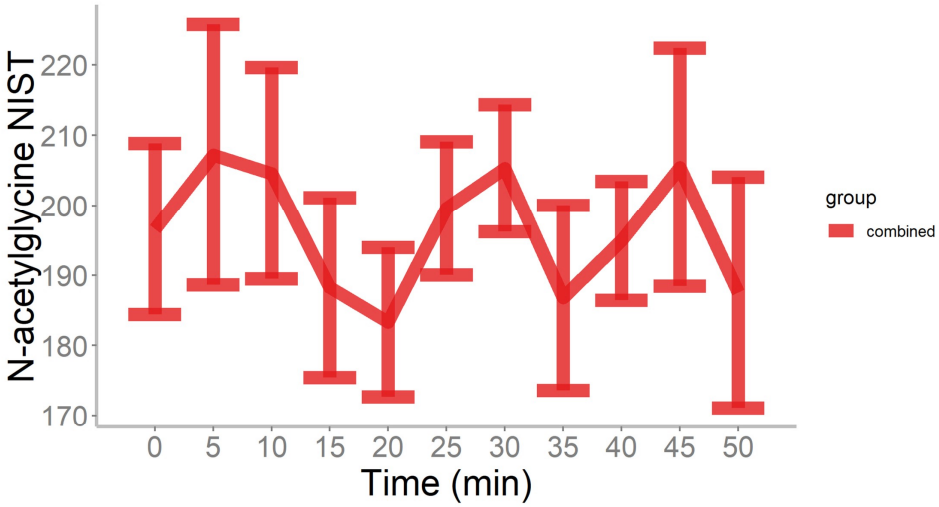

mannose
10000
5000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

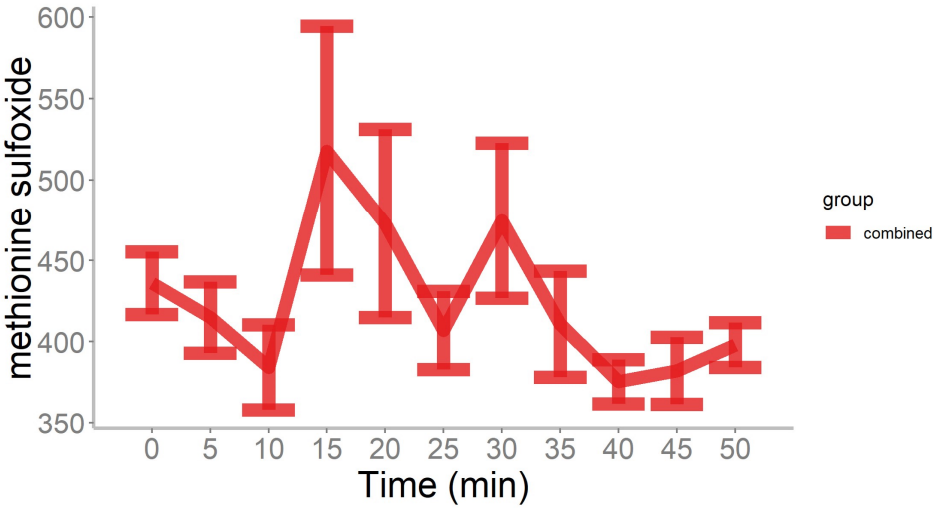

methionine
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

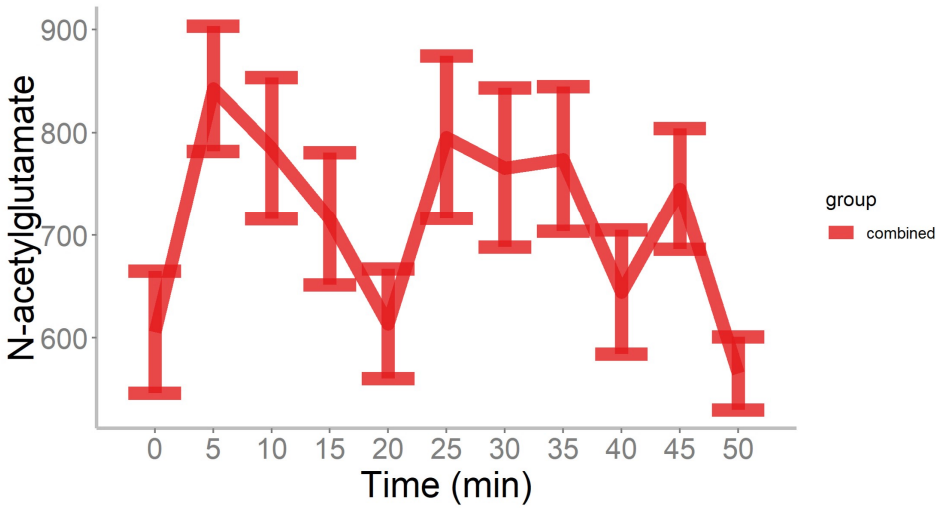

mannitol
4000
3000
2000
1000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

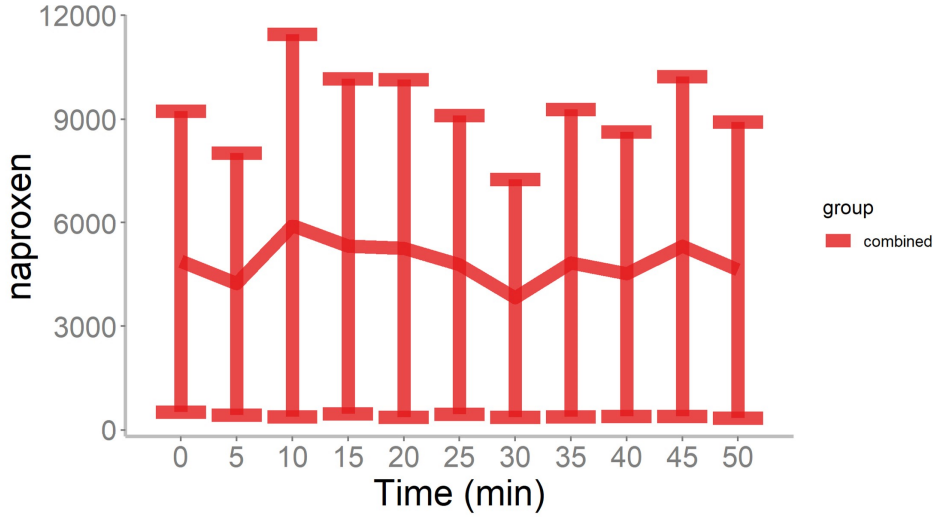

methanolphosphate
1200
1100
1000
900
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

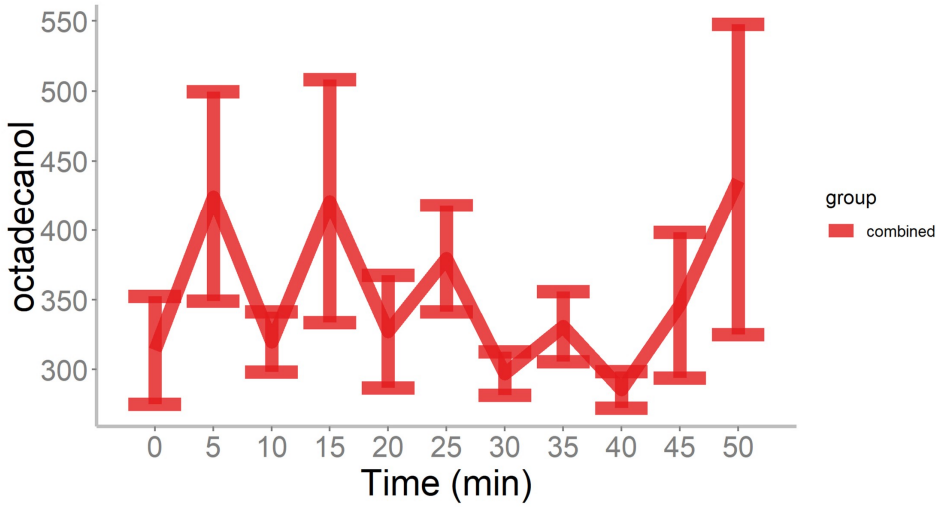

myristic acid
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

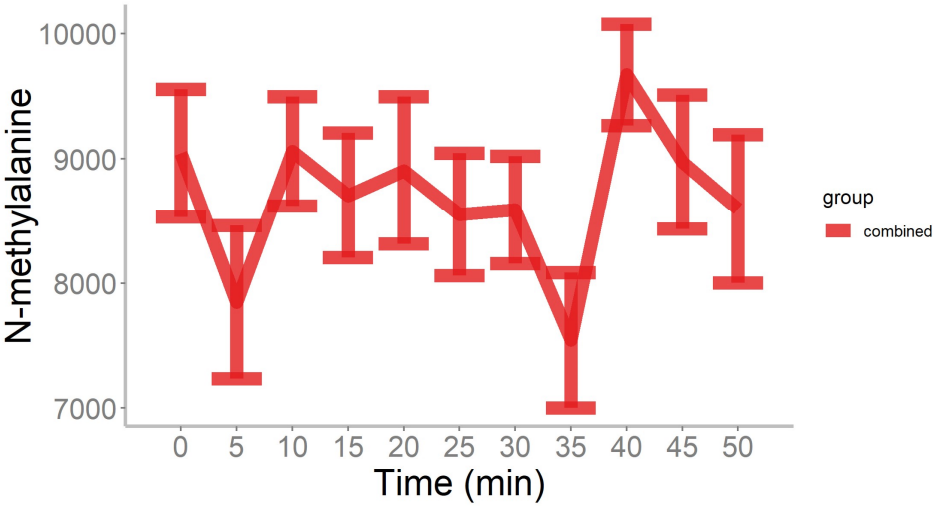

N-acetylglycine NIST
220
210
200
190
180
170
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

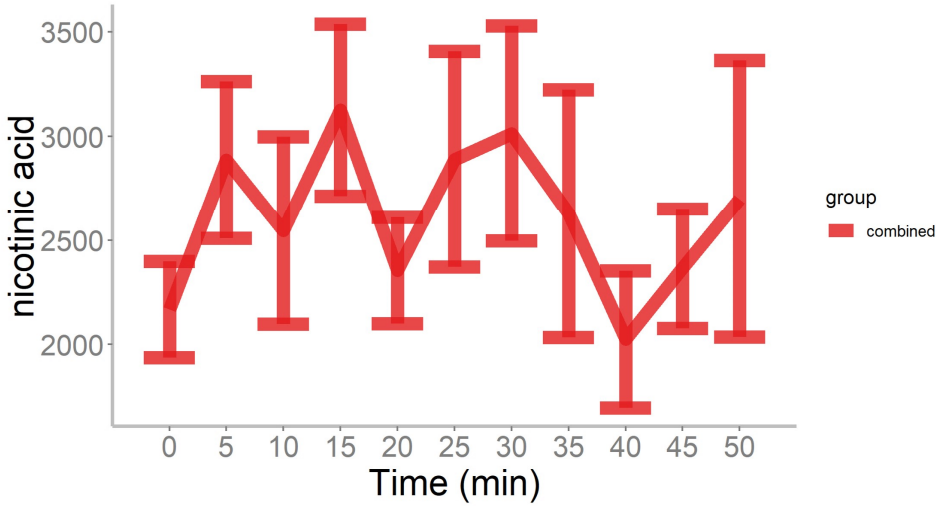

methionine sulfoxide
600
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

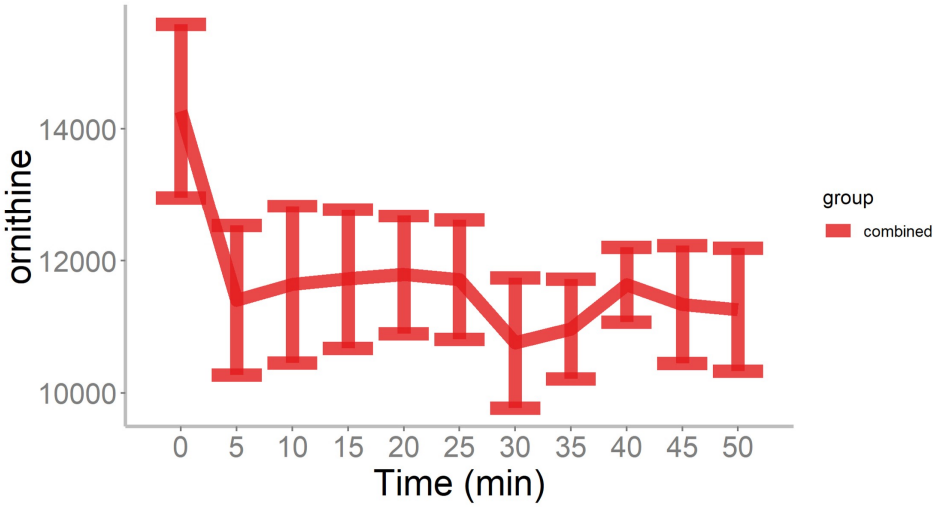

N-acetylglutamate
900
800
700
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

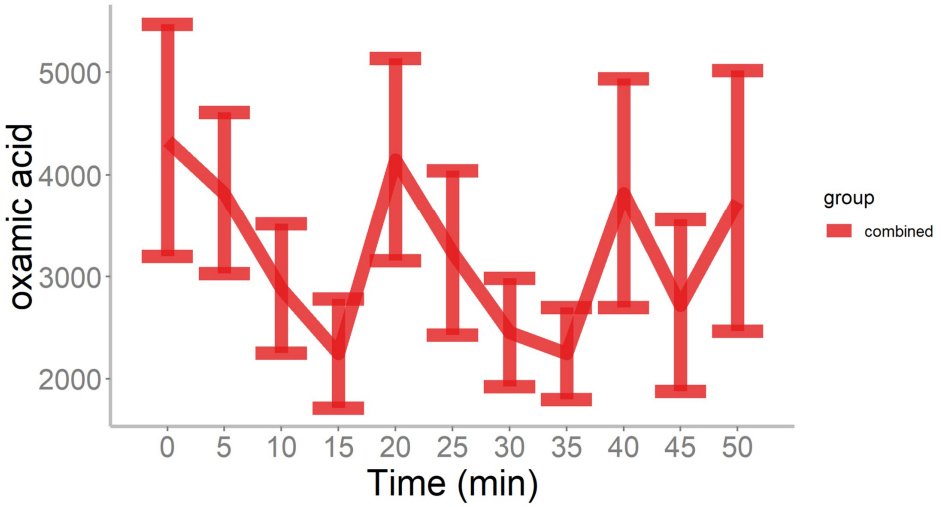

naproxen
12000
9000
6000
3000
0
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

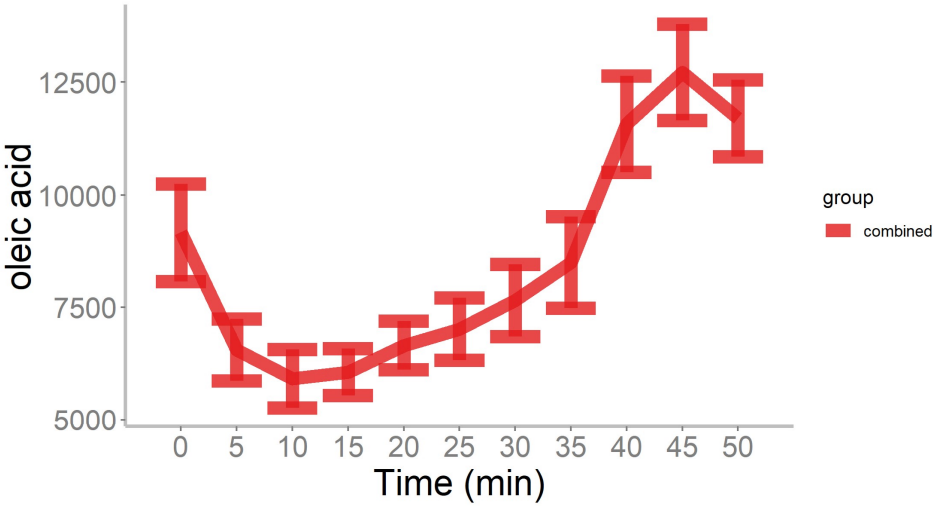

octadecanol
550
500
450
400
350
300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


N-methylalanine
10000
9000
8000
7000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


nicotinic acid
3500
3000
2500
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


ornithine
14000
12000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


oxamic acid
5000
4000
3000
2000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


oleic acid
12500
10000
7500
5000
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Time (min)
group
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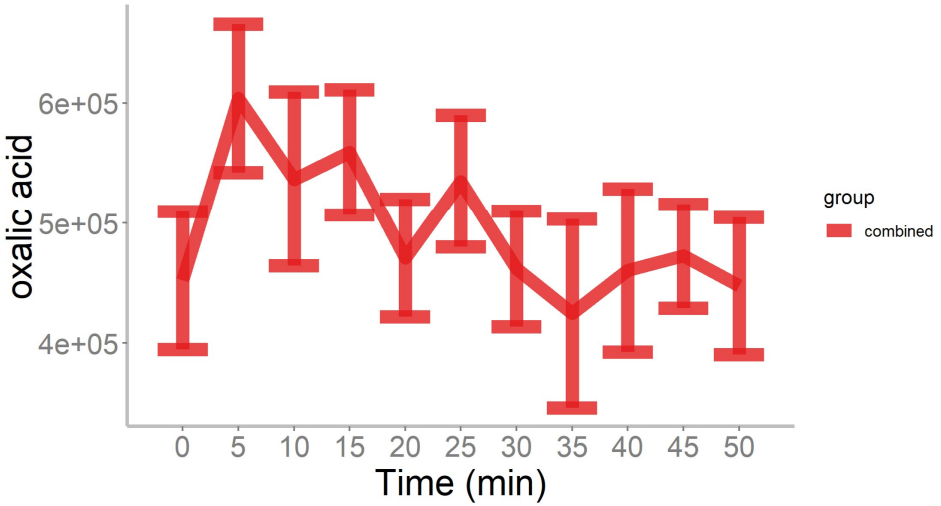
oxalic acid
6e+05
5e+05
4e+05
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Time (min)
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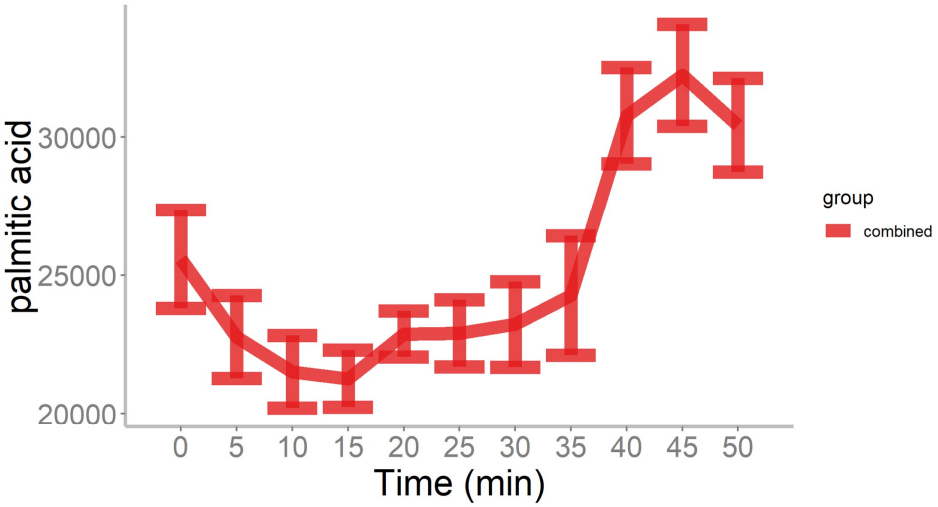
palmitic acid
30000
25000
20000
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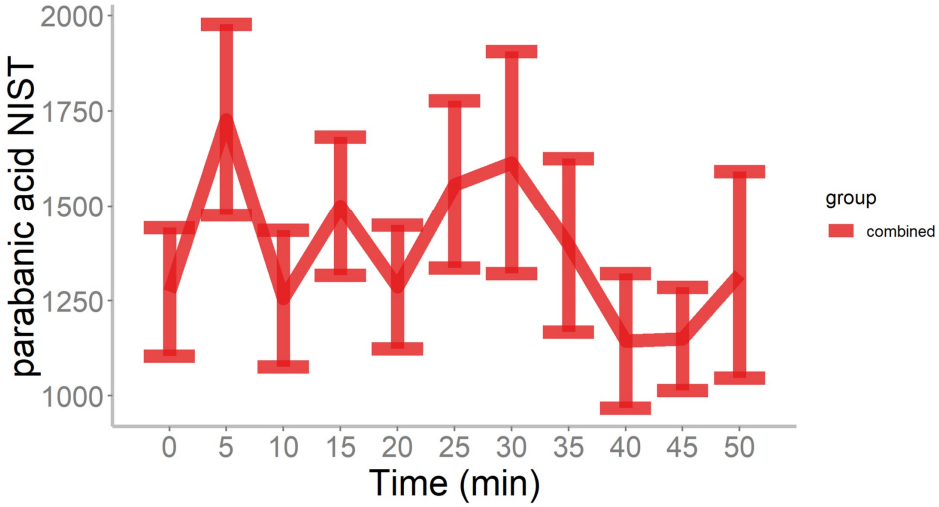
Time (min)
group
combined


parabanic acid NIST
2000
1750
1500
1250
1000
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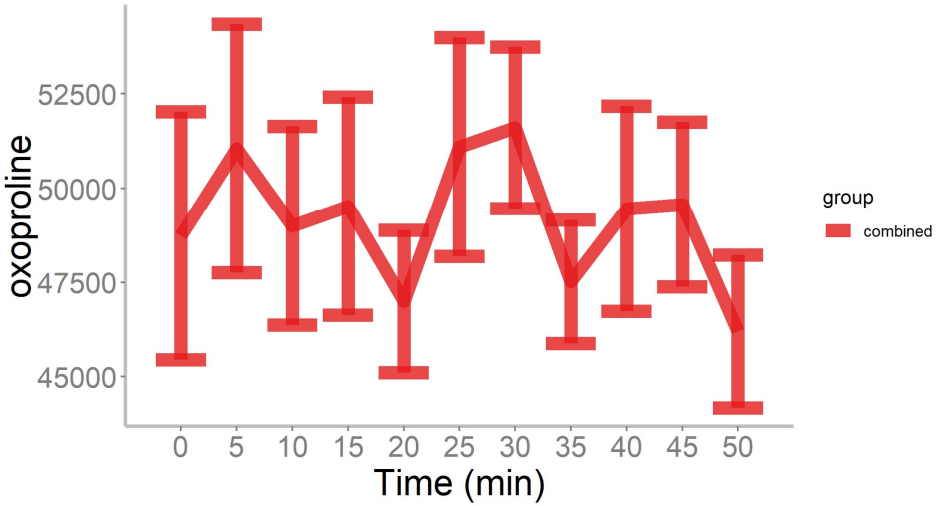
Time (min)
group
combined


oxoproline
52500
50000
47500
45000
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Time (min)
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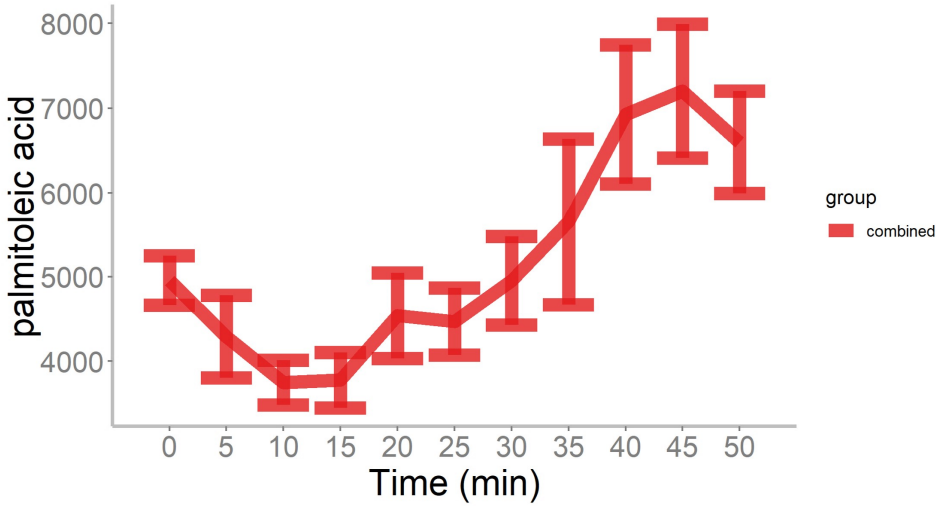
palmitoleic acid
8000
7000
6000
5000
4000
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Time (min)
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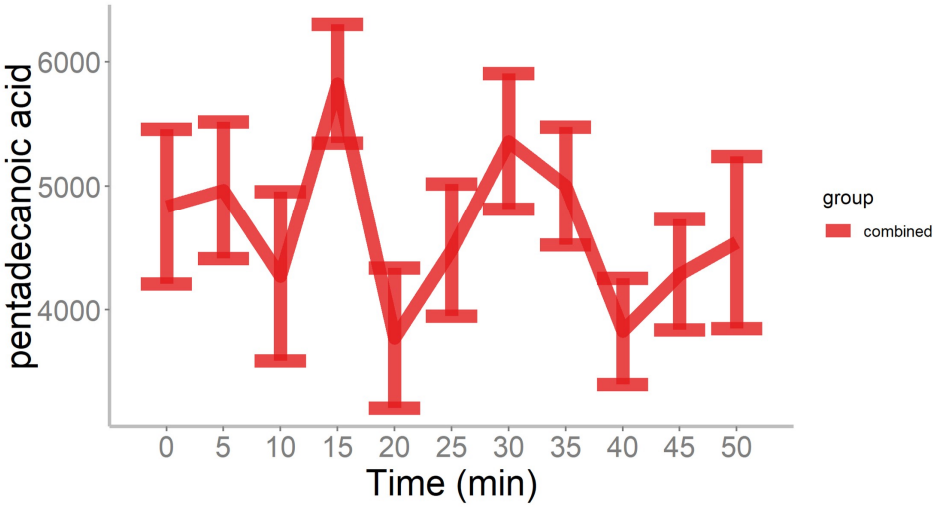
pentadecanoic acid
6000
5000
4000
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Time (min)
group
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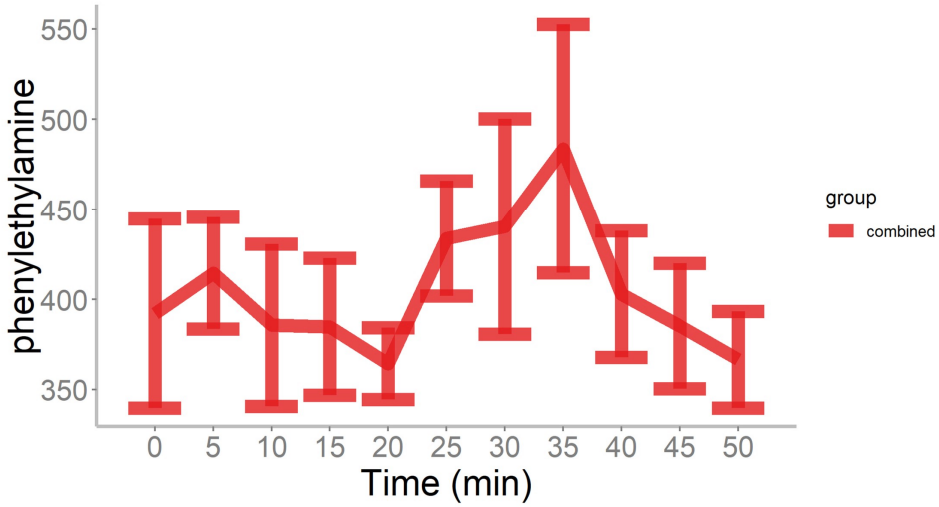
phenylethylamine
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
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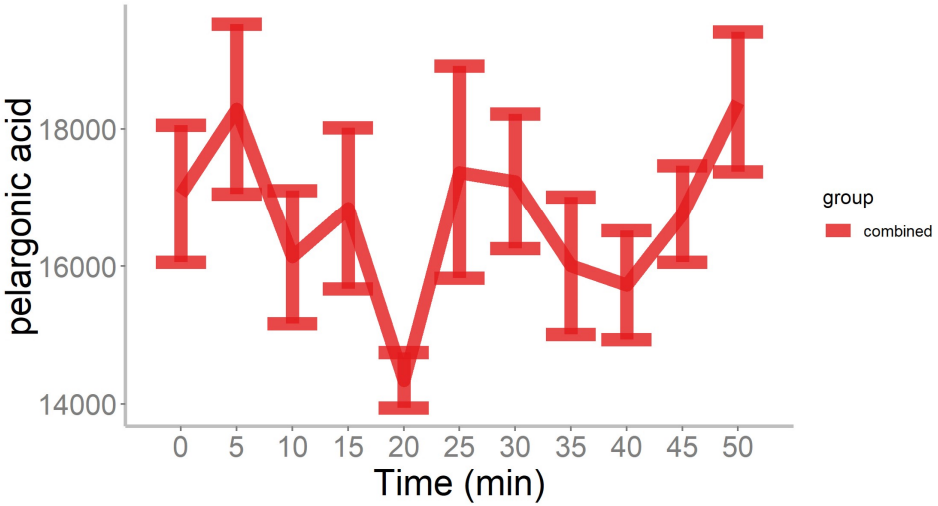
pelargonic acid
18000
16000
14000
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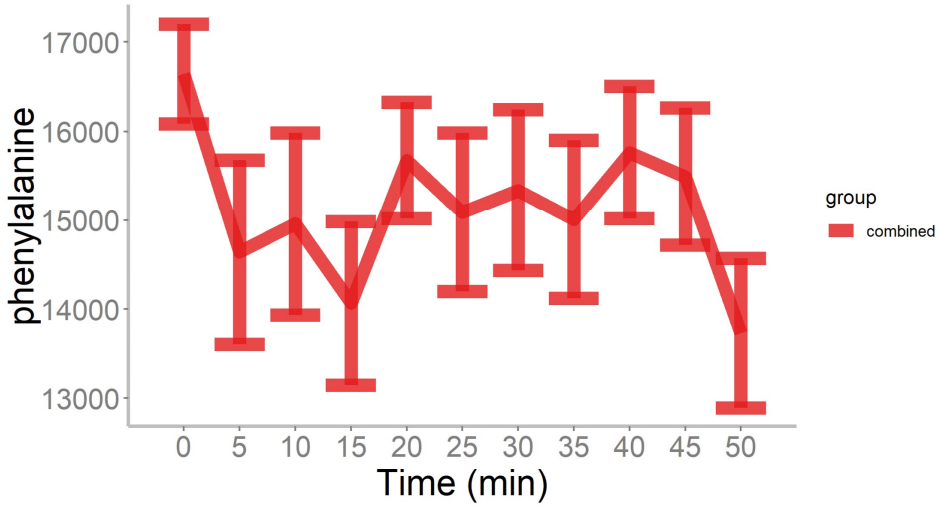
Time (min)
group
combined


phenylalanine
17000
16000
15000
14000
13000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
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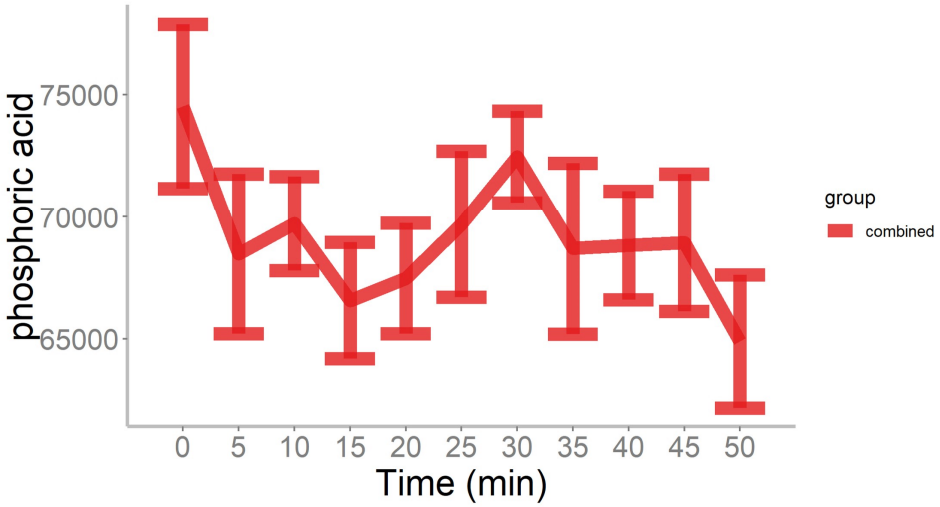
phosphoric acid
75000
70000
65000
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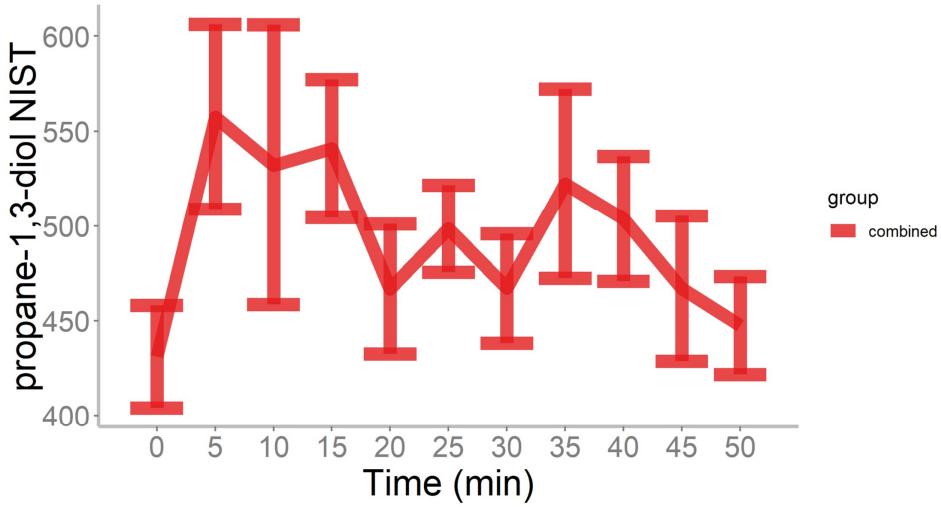
Time (min)
group
combined


propane-1,3-diol NIST
600
550
500
450
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
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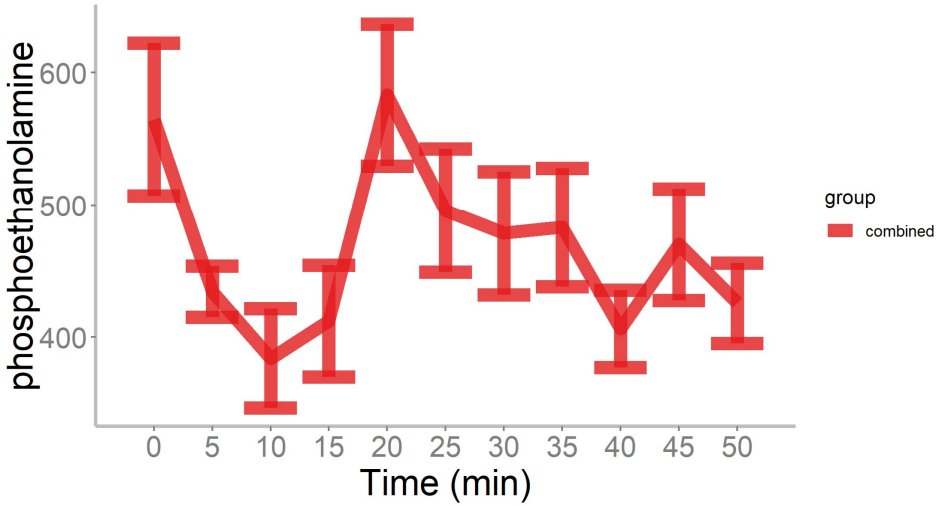
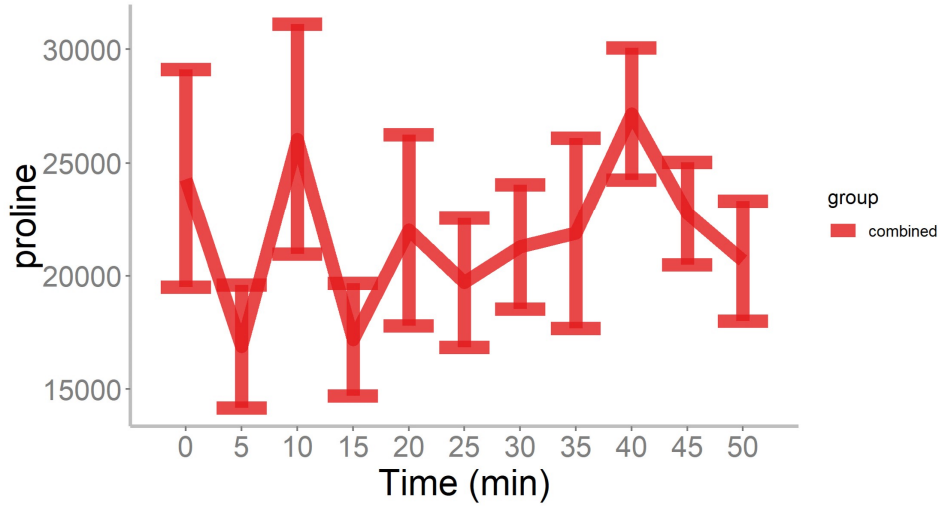
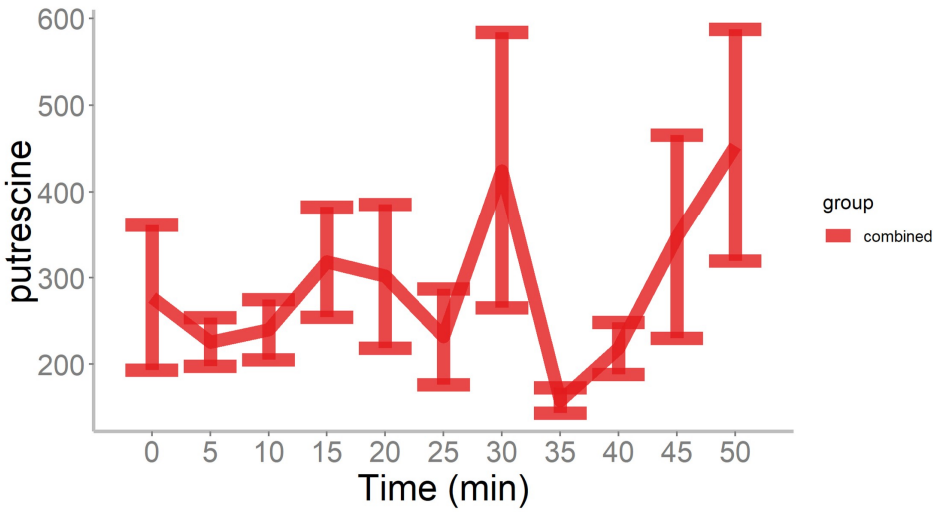
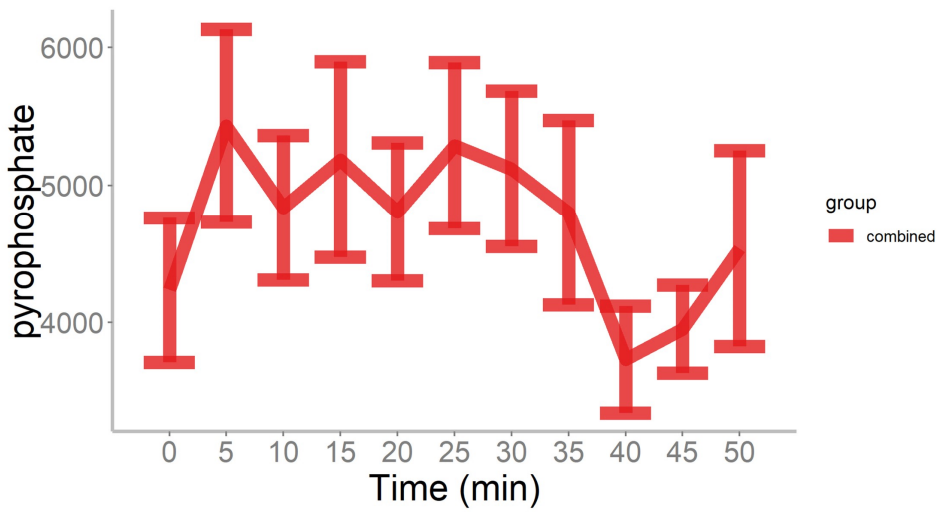
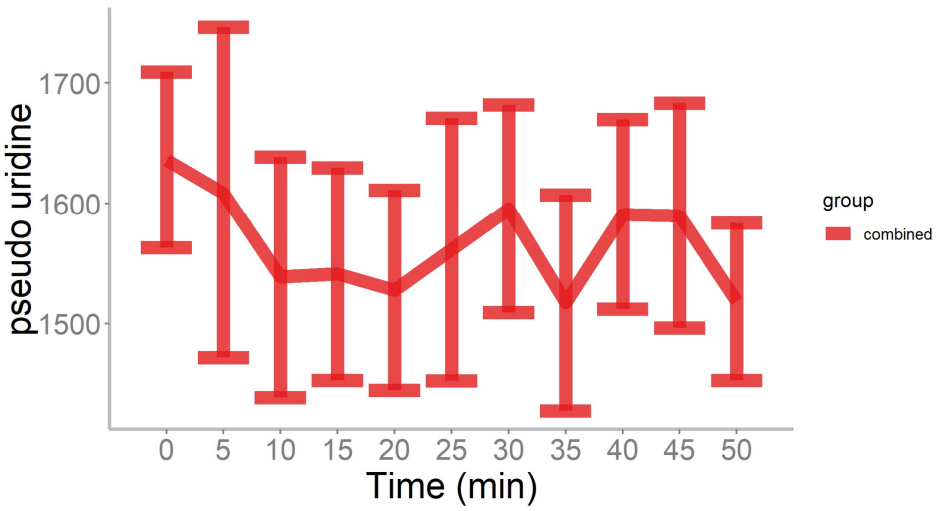
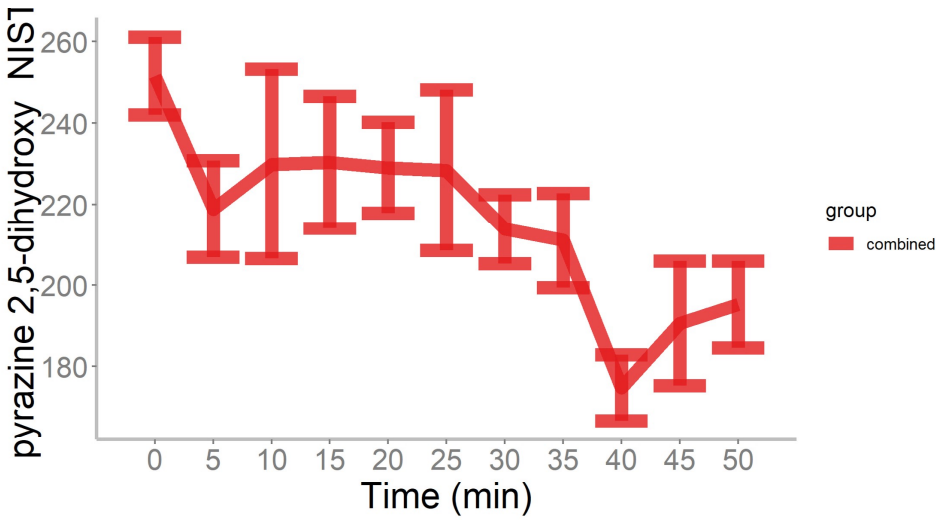

phosphoethanolamine
600
500
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

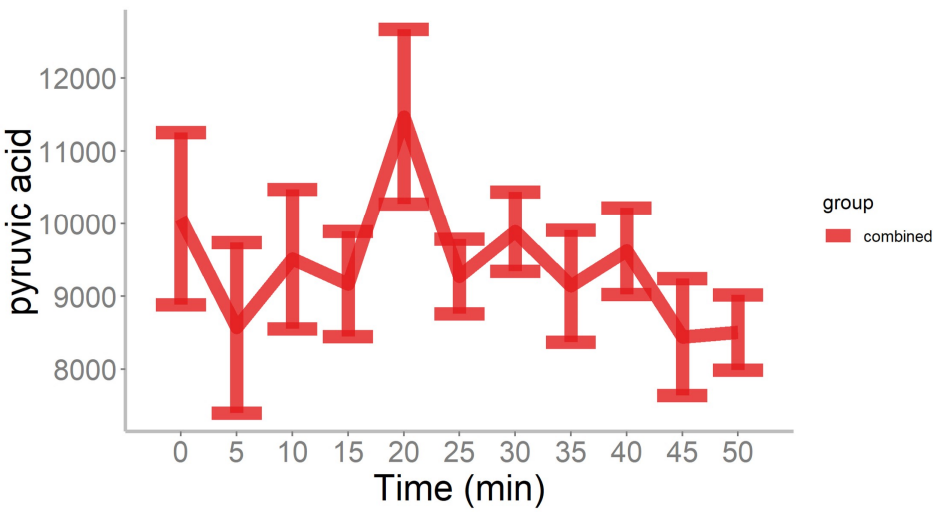

proline
30000
25000
20000
15000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

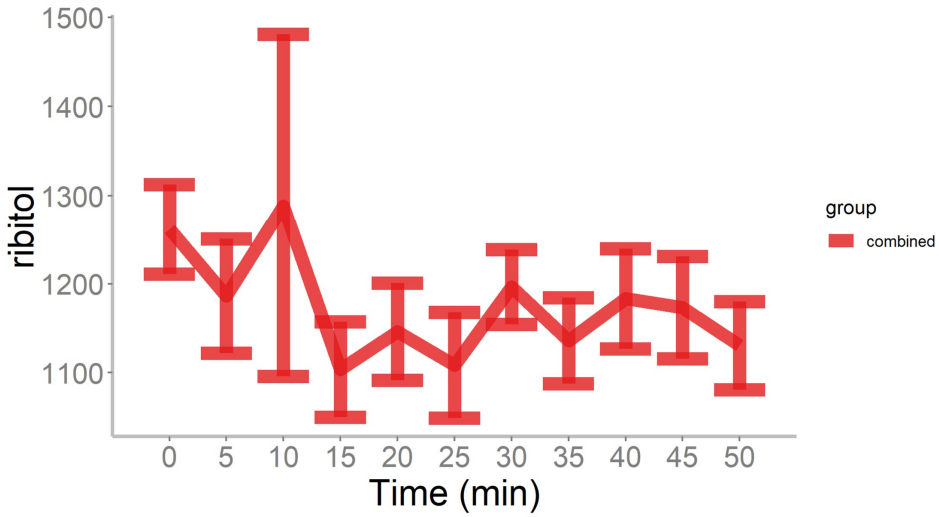

putrescine
600
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

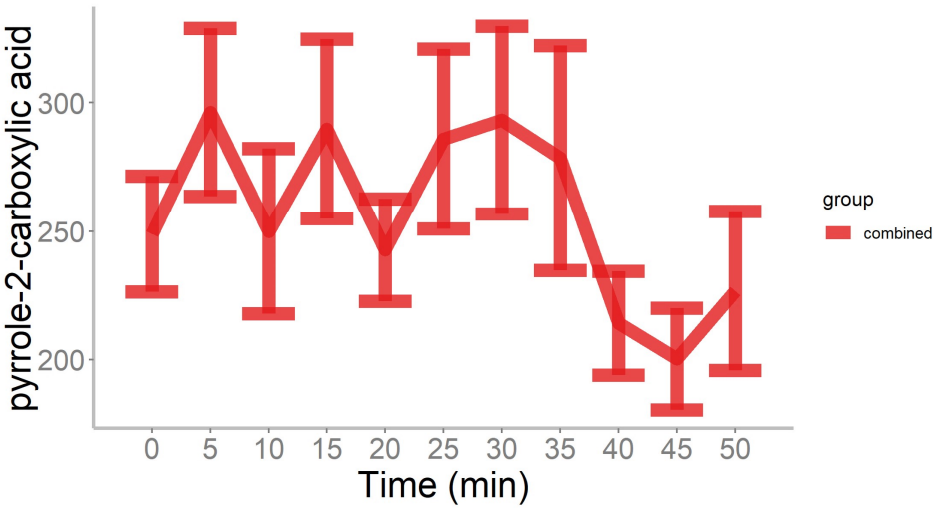

pyrophosphate
6000
5000
4000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


pseudo uridine
1700
1600
1500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


pyrazine 2,5-dihydroxy NIST
260
240
220
200
180
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


pyruvic acid
12000
11000
10000
9000
8000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


ribitol
1500
1400
1300
1200
1100
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


pyrrole-2-carboxylic acid
300
250
200
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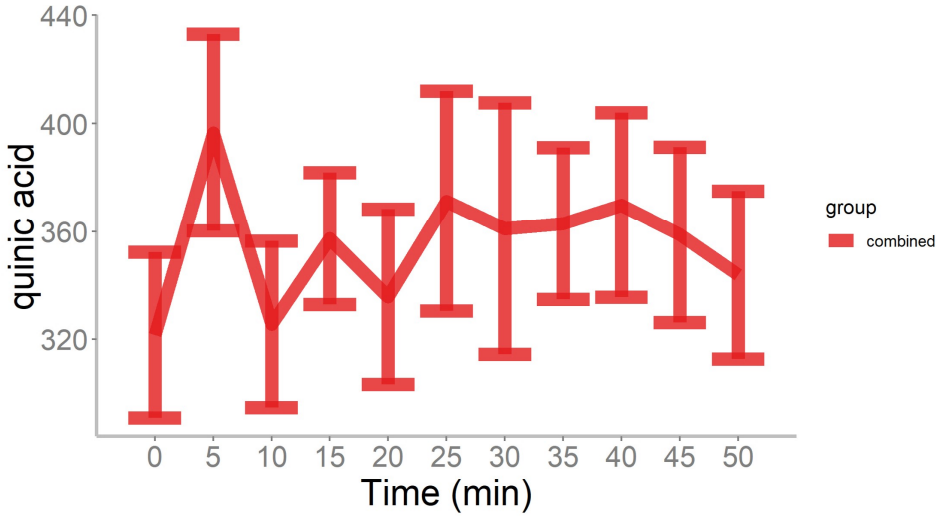
Time (min)
group
combined


quinic acid
440
400
360
320
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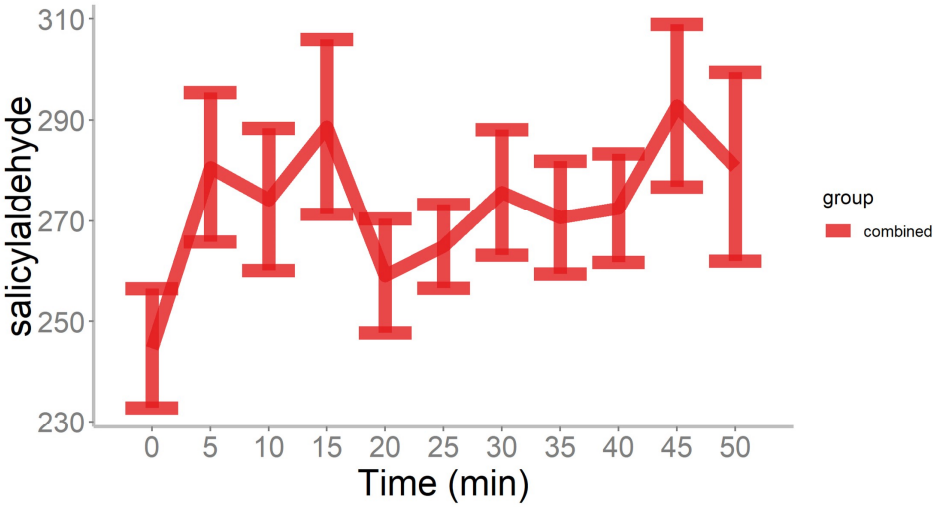
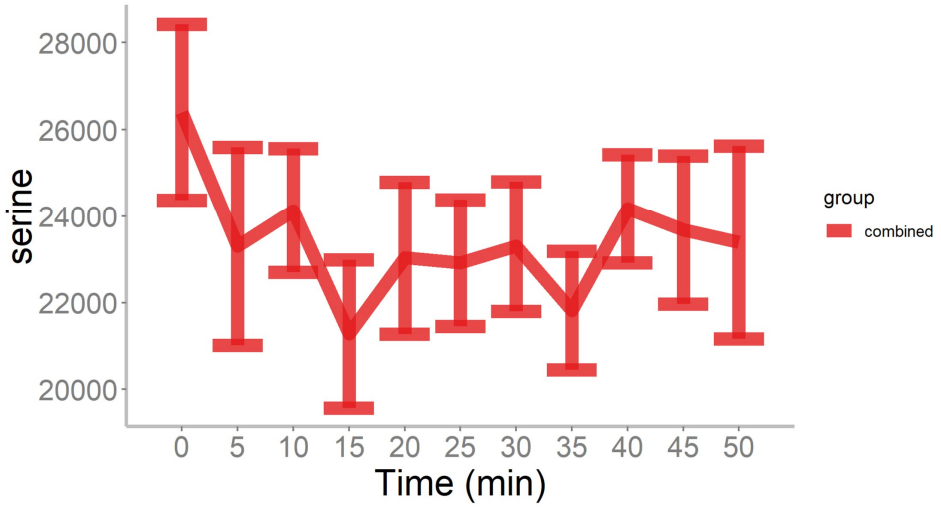
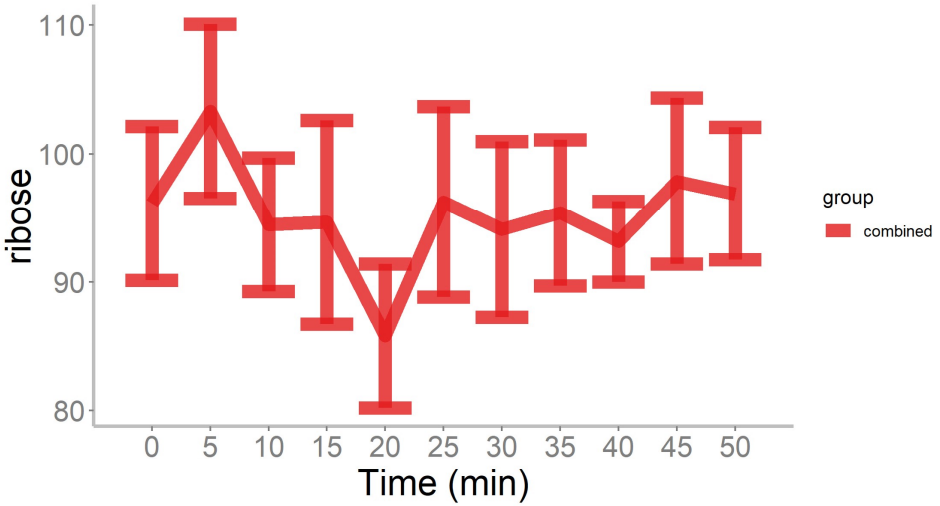
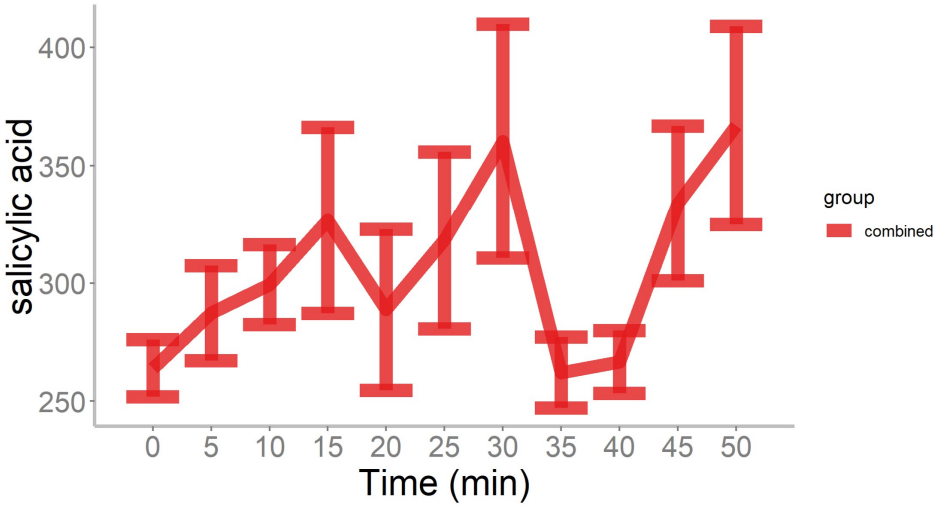
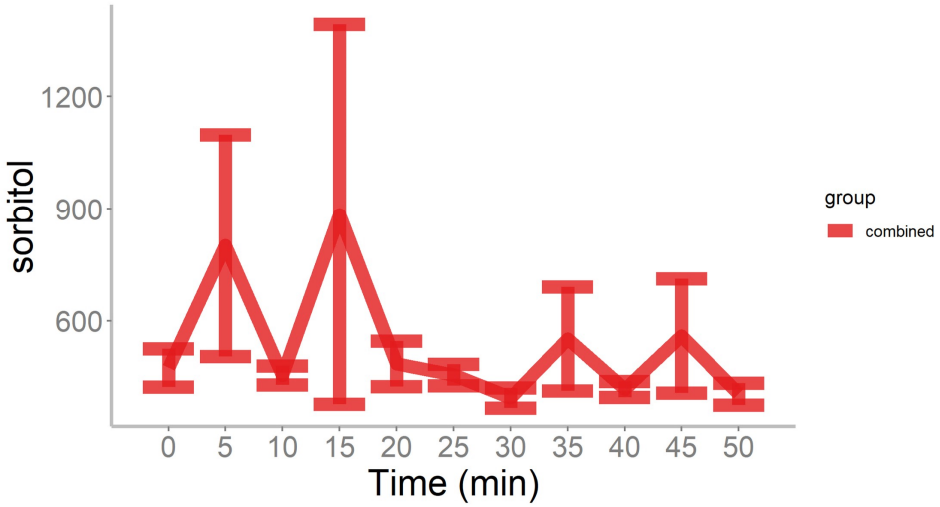
Time (min)
group
combined

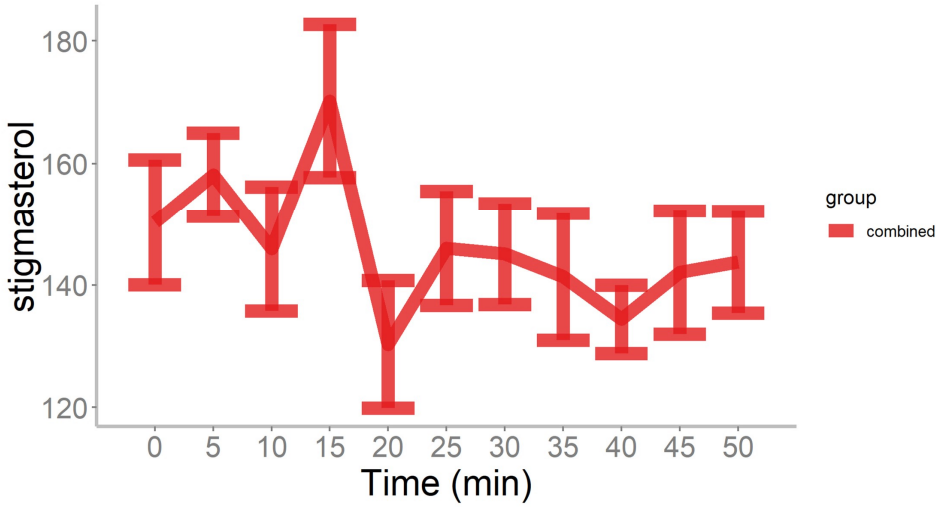

salicylaldehyde
310
290
270
250
230
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

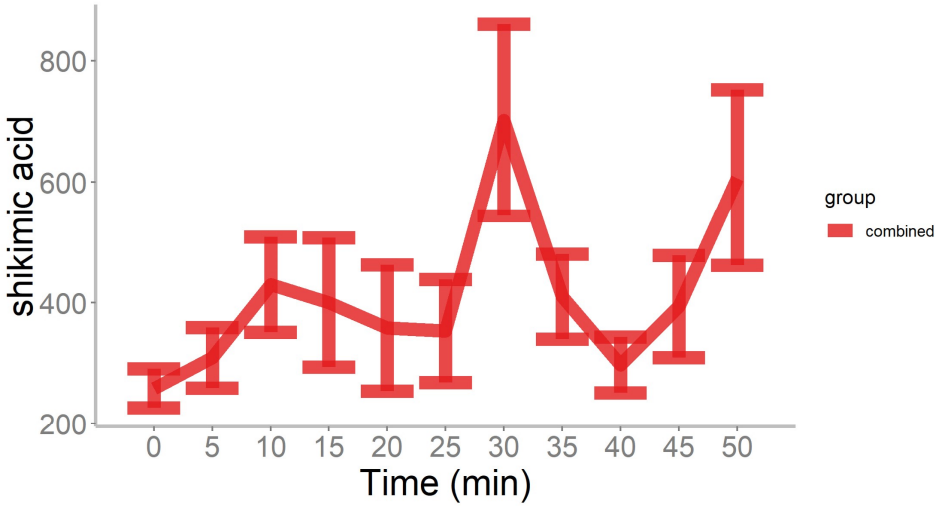

serine
28000
26000
24000
22000
20000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


ribose
110
100
90
80
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


salicylic acid
400
350
300
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


sorbitol
1200
900
600
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


stigmasterol
180
160
140
120
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


shikimic acid
800
600
400
200
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Time (min)
group
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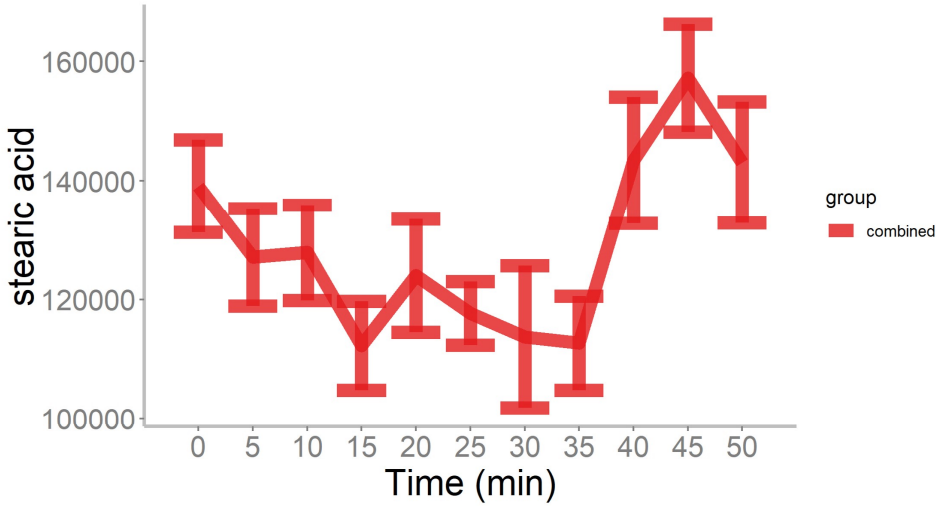
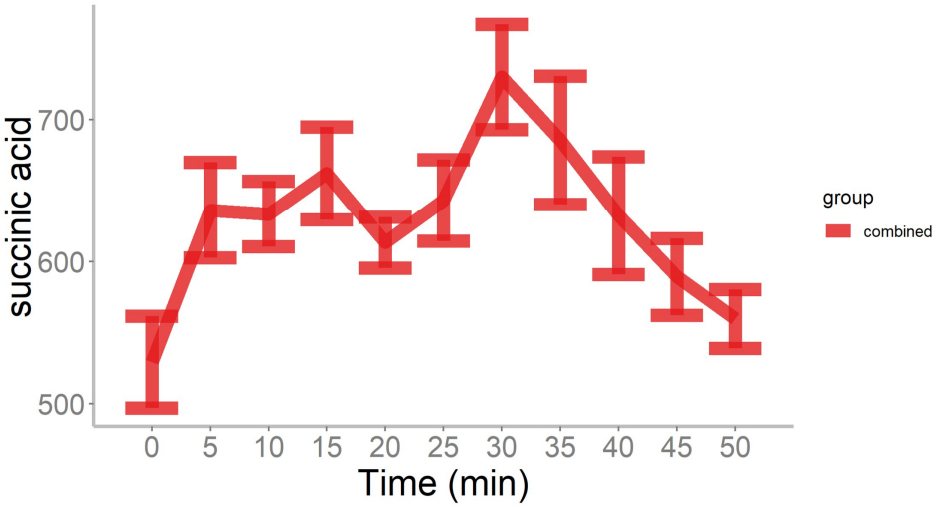
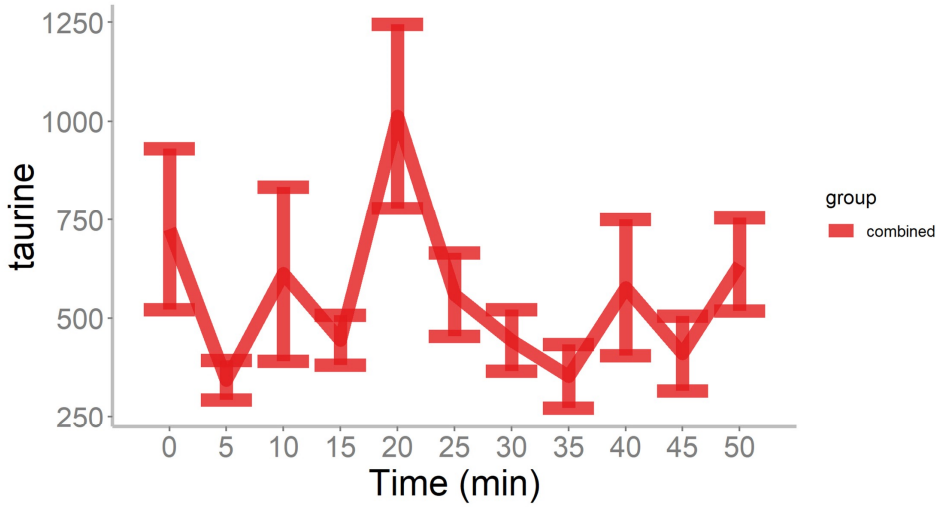
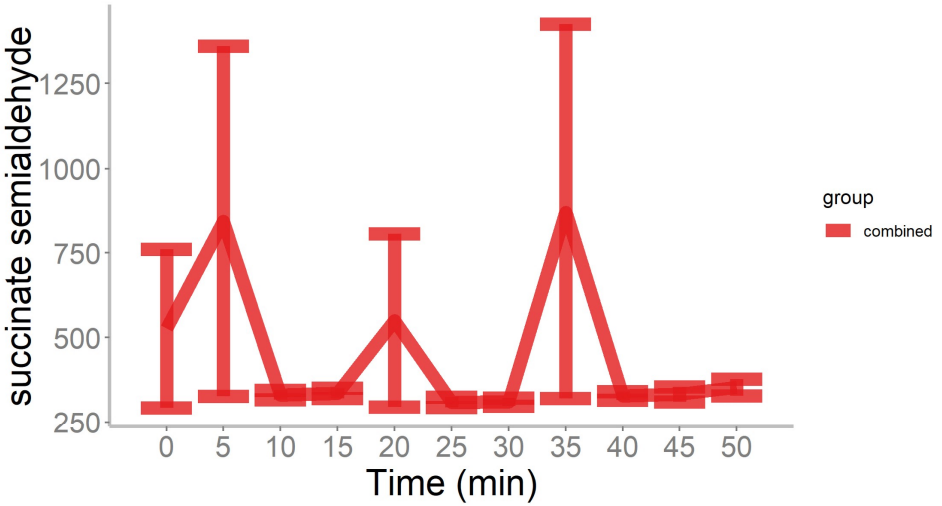
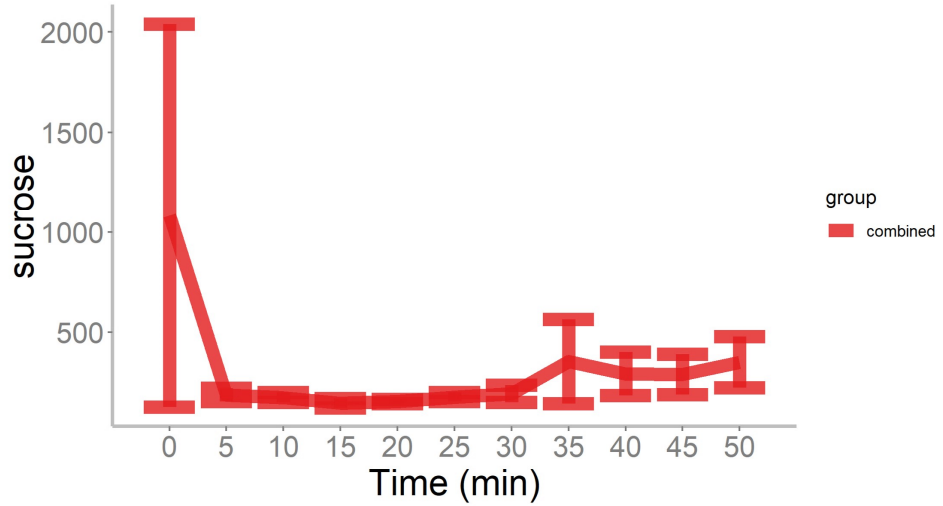
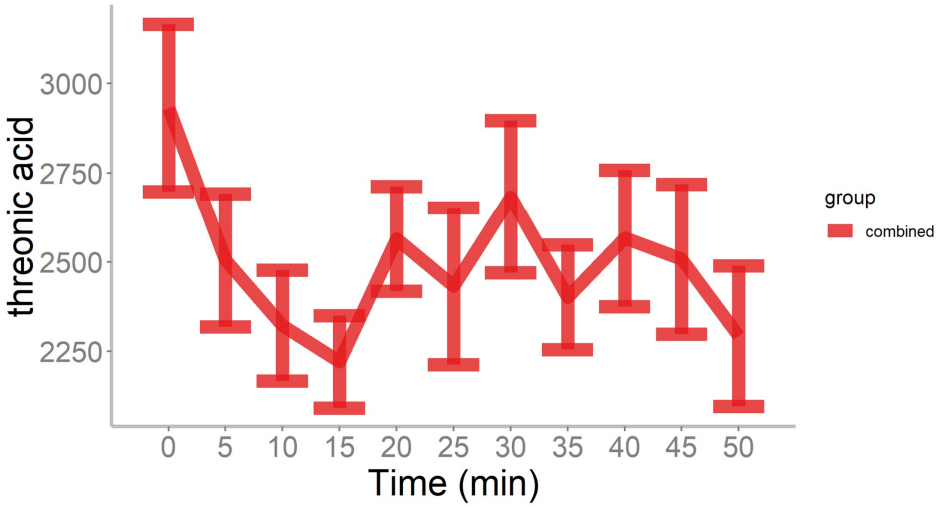

stearic acid
160000
140000
120000
100000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

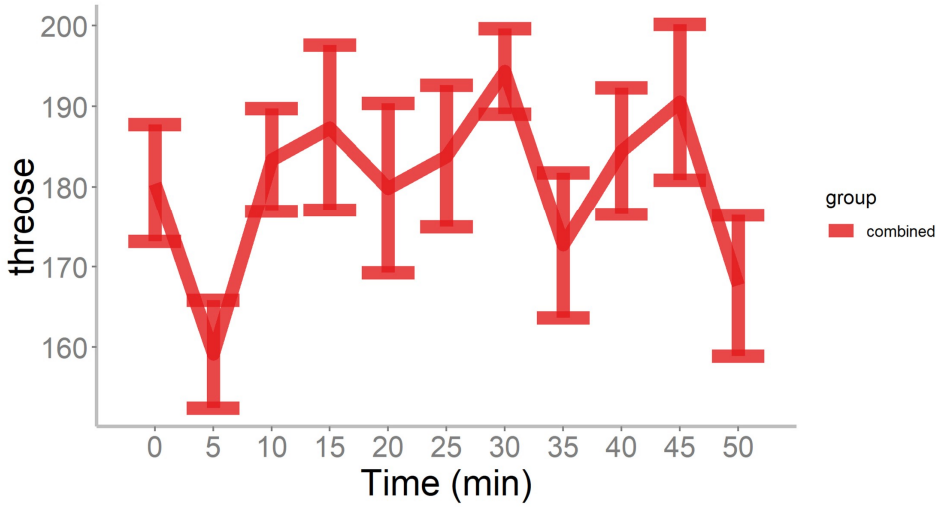

succinic acid
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

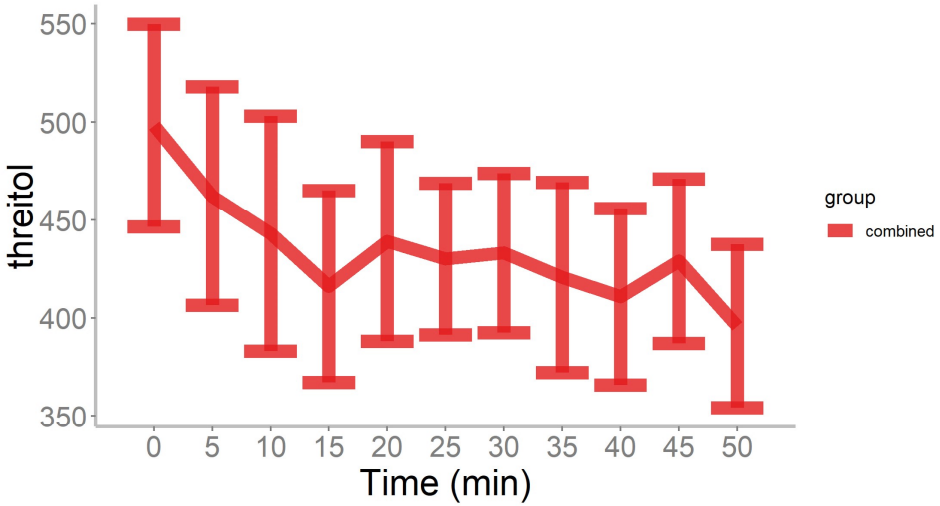

taurine
1250
1000
750
500
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

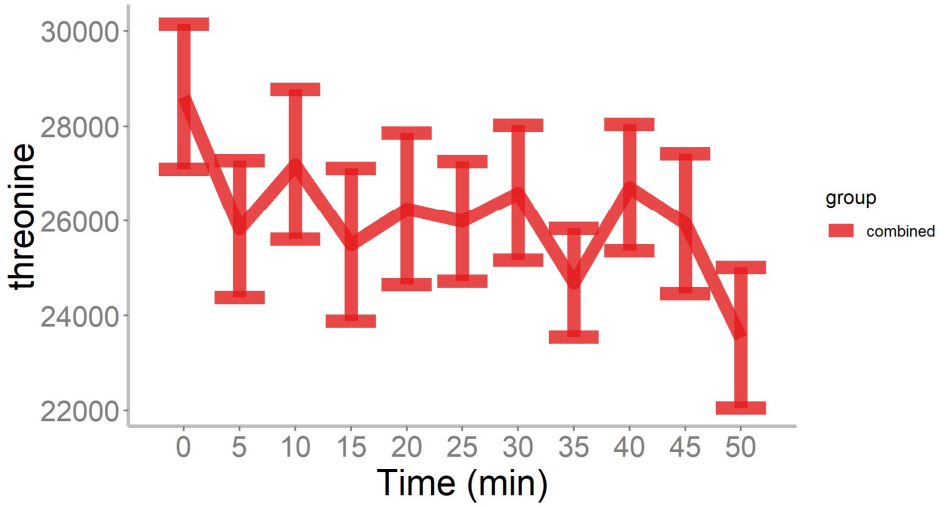

succinate semialdehyde
1250
1000
750
500
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

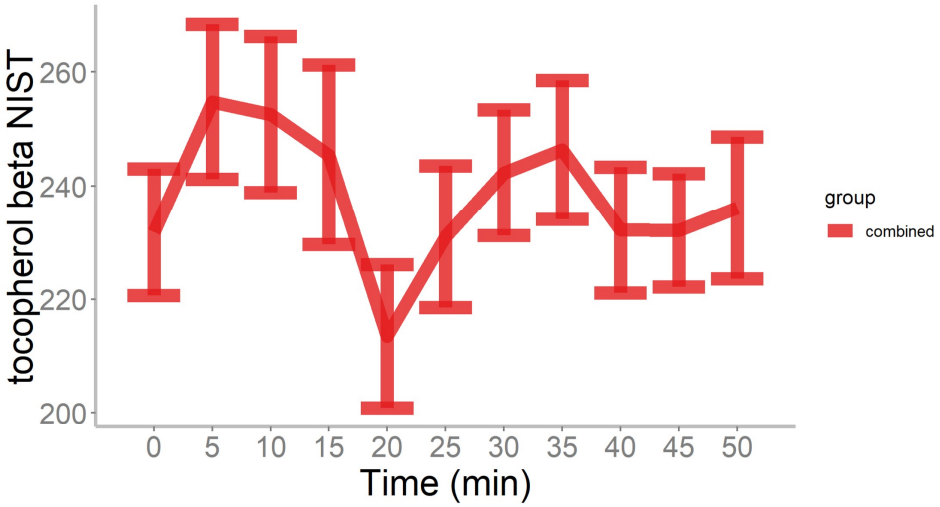

sucrose
2000
1500
1000
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

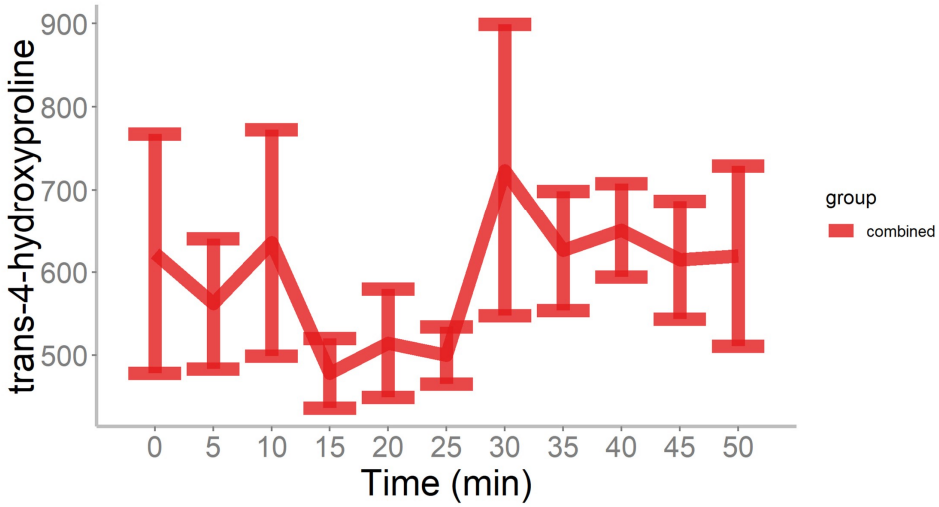

threonic acid
3000
2750
2500
2250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

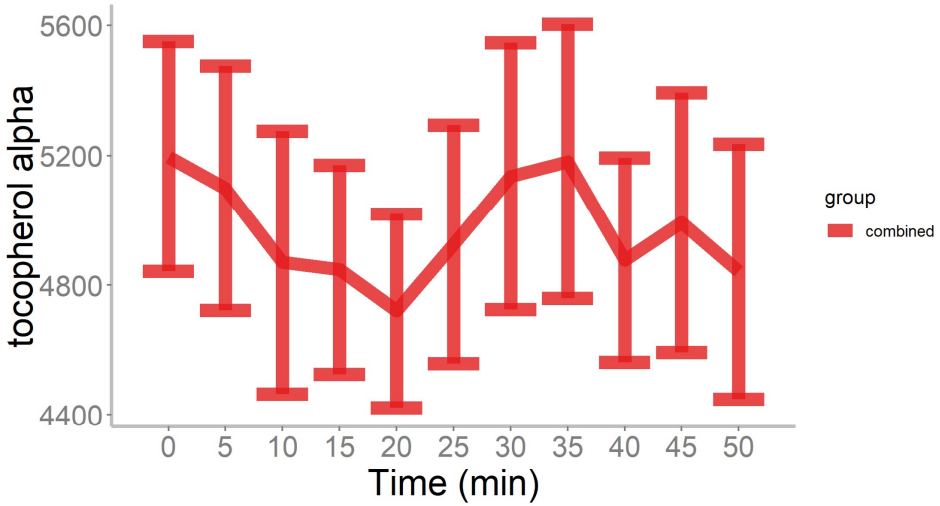

threose
200
190
180
170
160
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

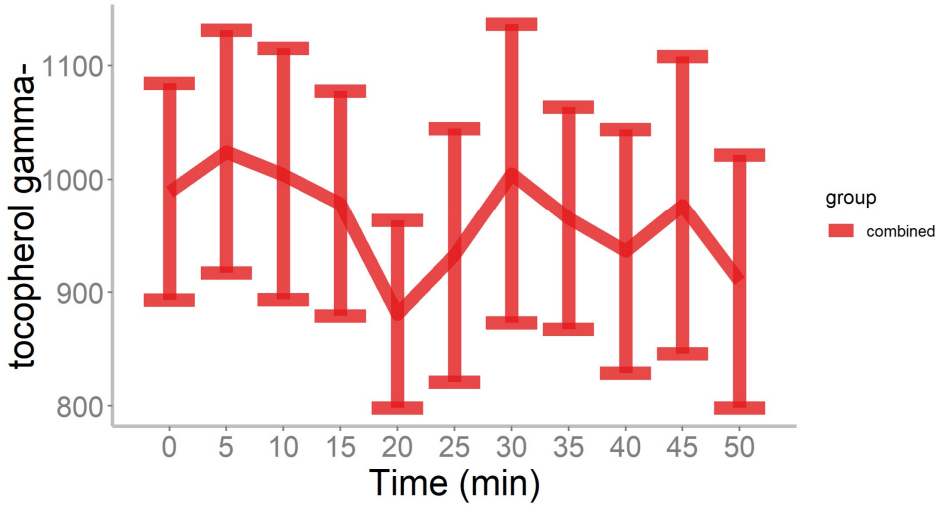

threitol
550
500
450
400
350
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

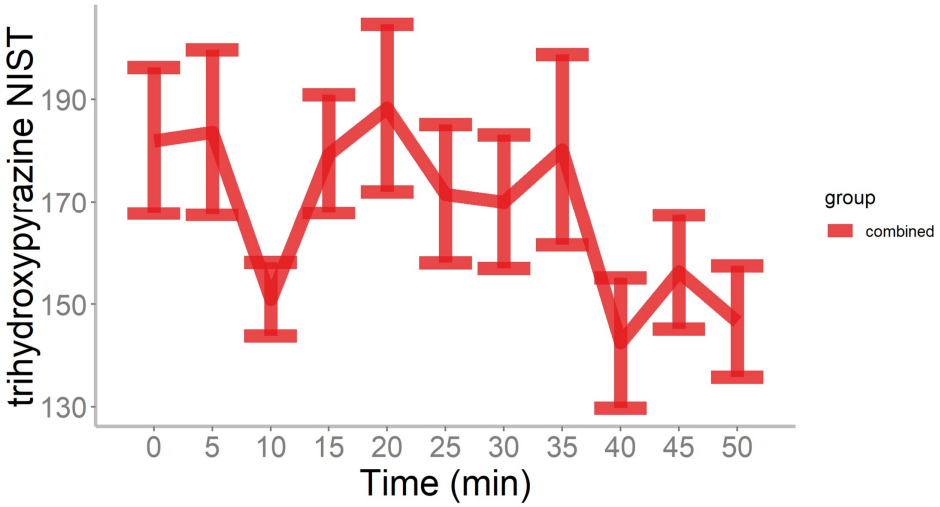

threonine
30000
28000
26000
24000
22000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

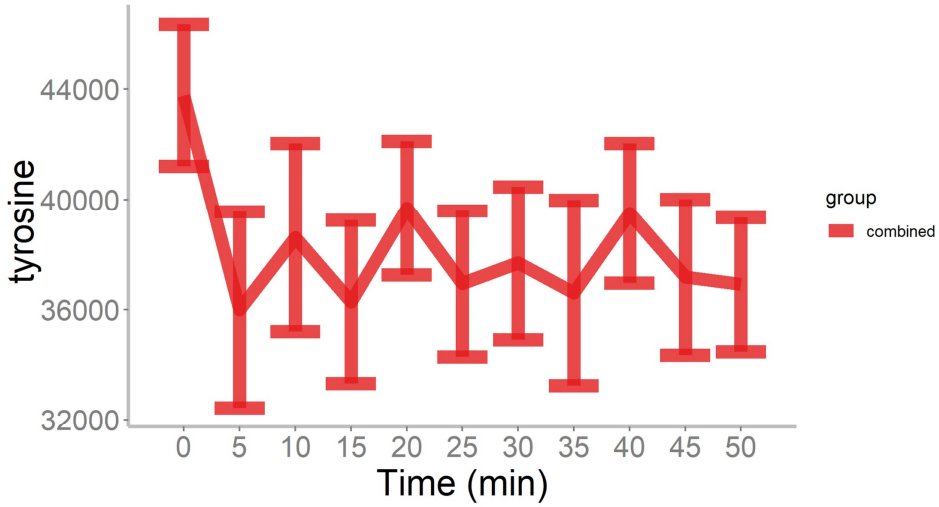

tocopherol beta NIST
260
240
220
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

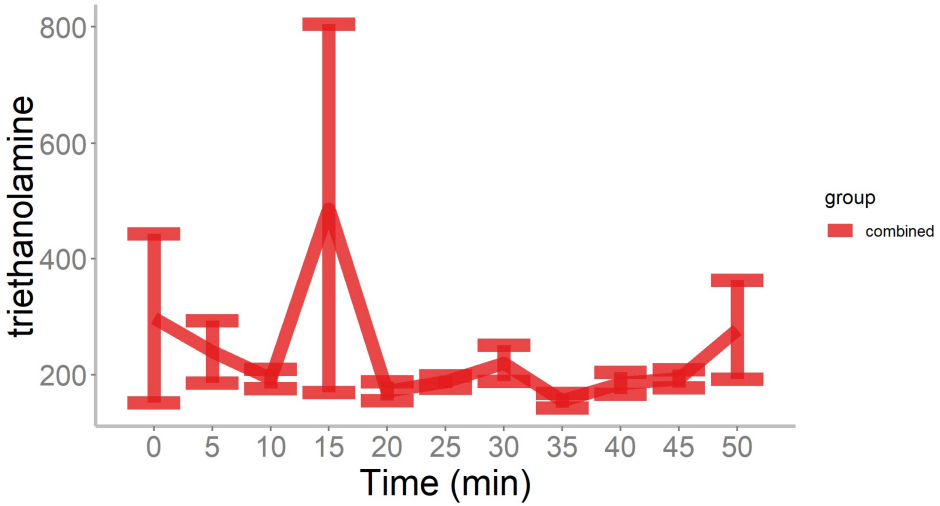

trans-4-hydroxyproline
900
800
700
600
500
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

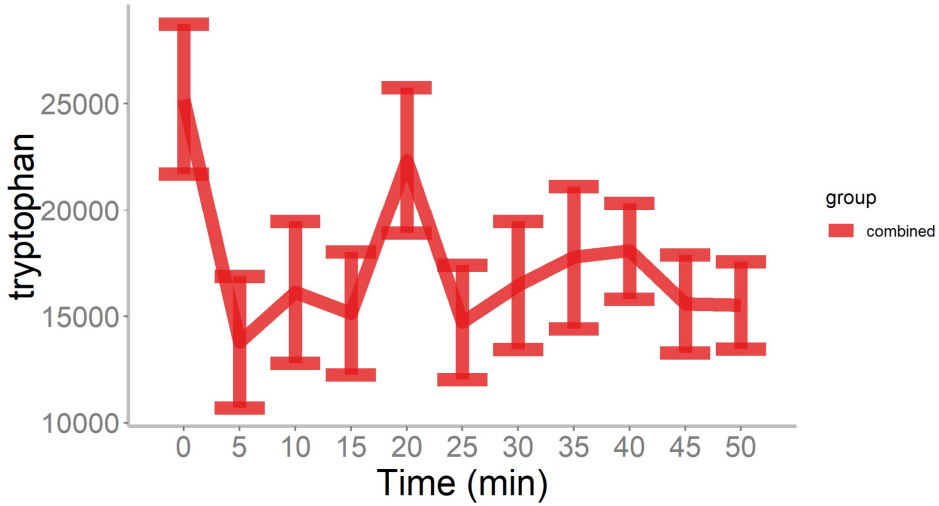

tocopherol alpha
5600
5200
4800
4400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

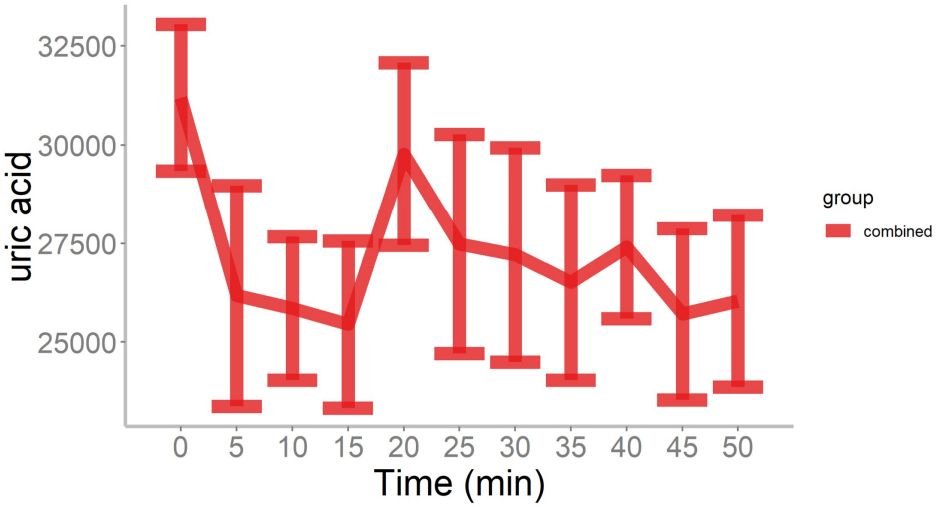

tocopherol gamma-
1100
1000
900
800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

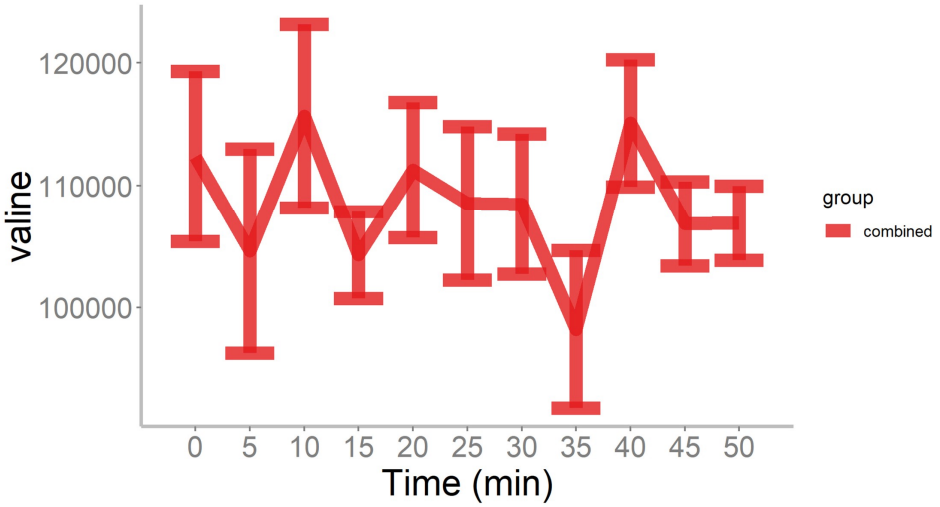

trihydroxypyrazine NIST
190
170
150
130
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

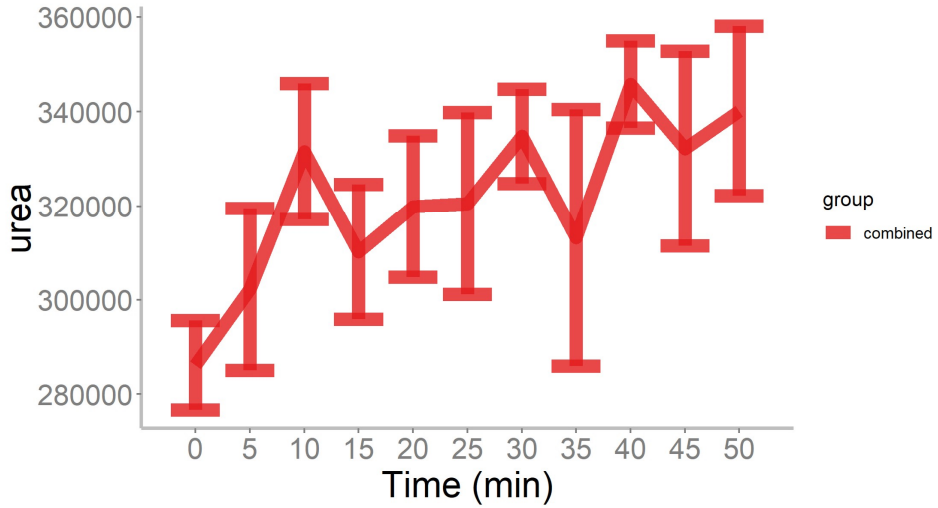

tyrosine
44000
40000
36000
32000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

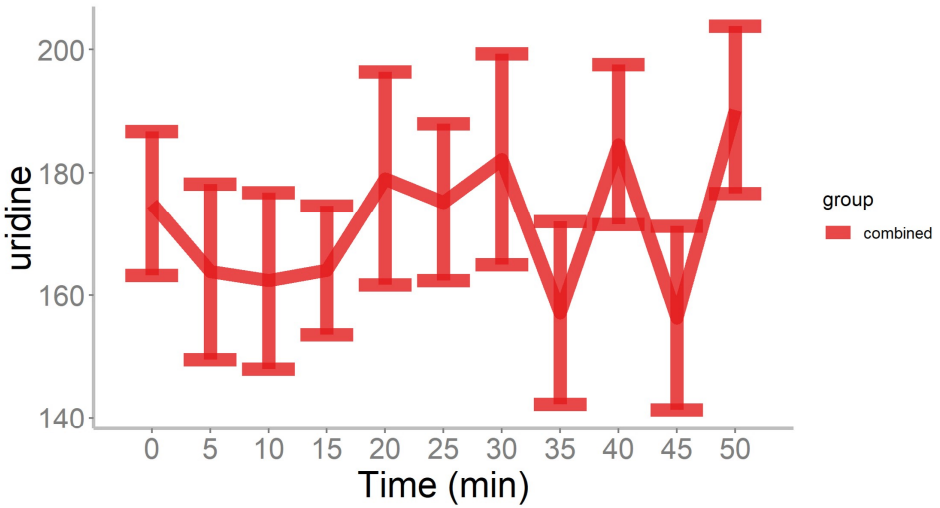

triethanolamine
800
600
400
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

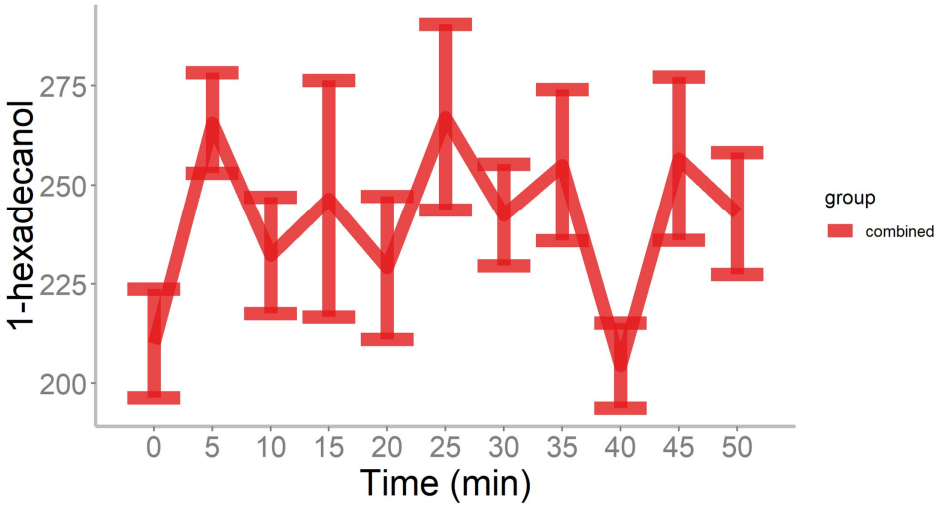

tryptophan
25000
20000
15000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

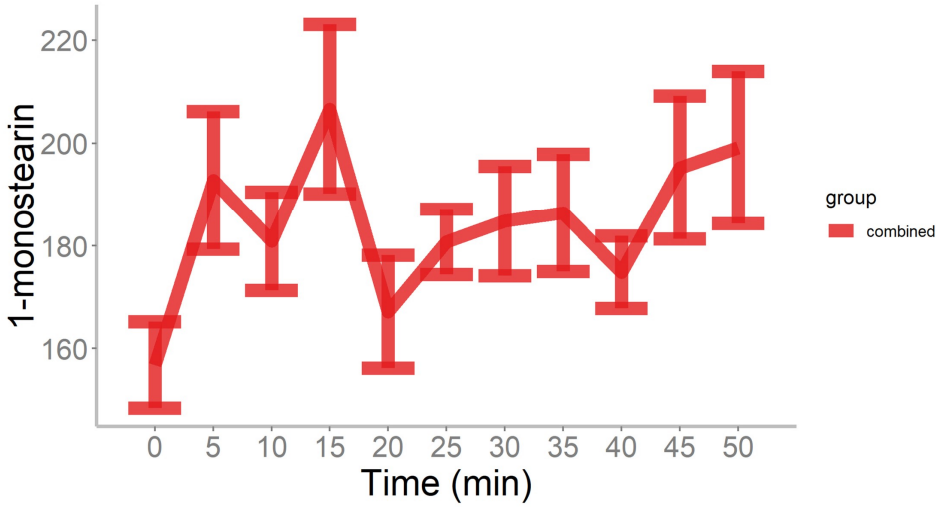

uric acid
32500
30000
27500
25000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

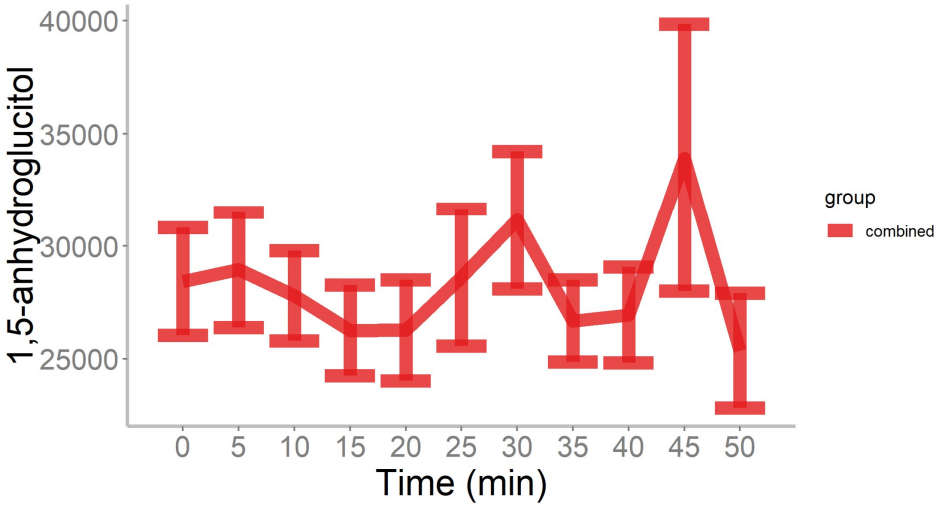

valine
120000
110000
100000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

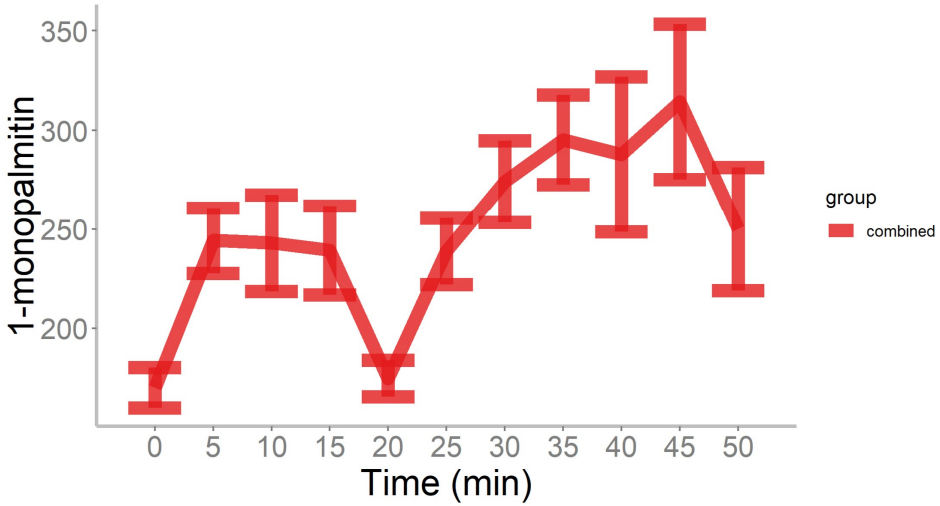

urea
360000
340000
320000
300000
280000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

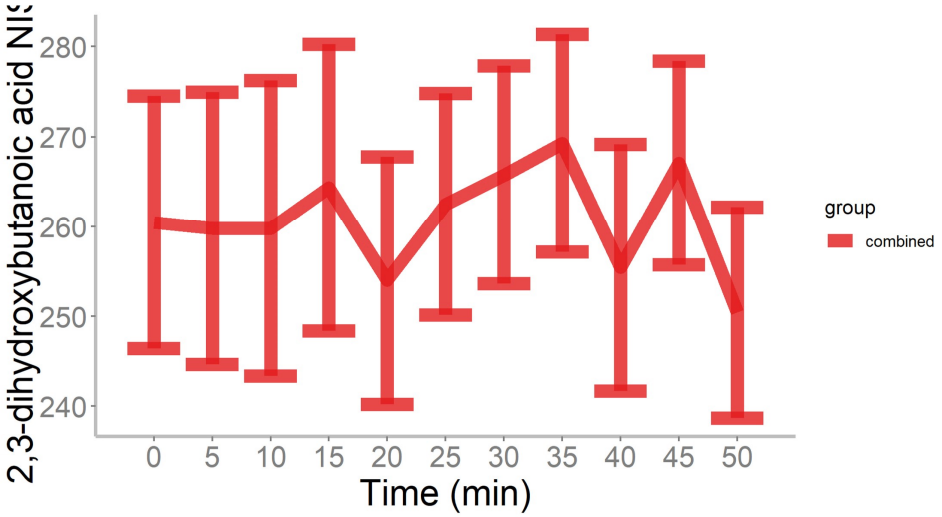

uridine
200
180
160
140
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

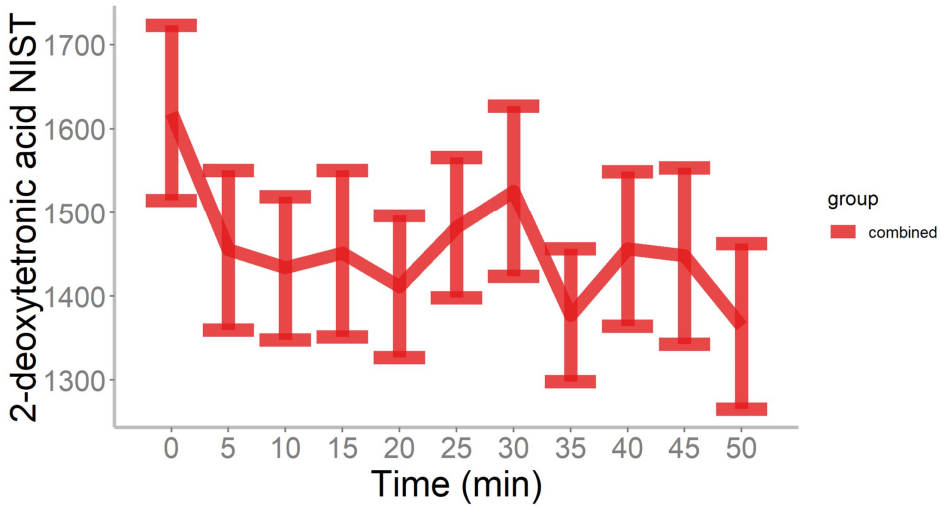

1-hexadecanol
275
250
225
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

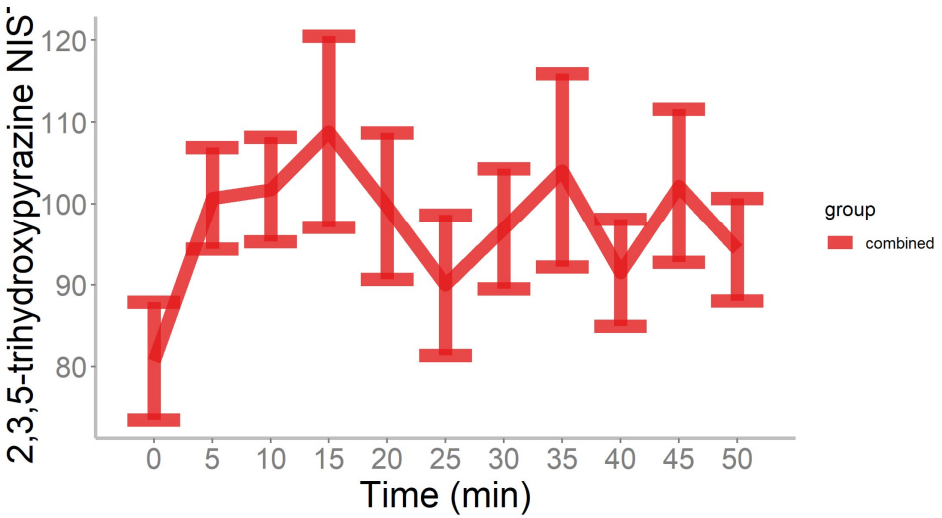

1-monostearin
220
200
180
160
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

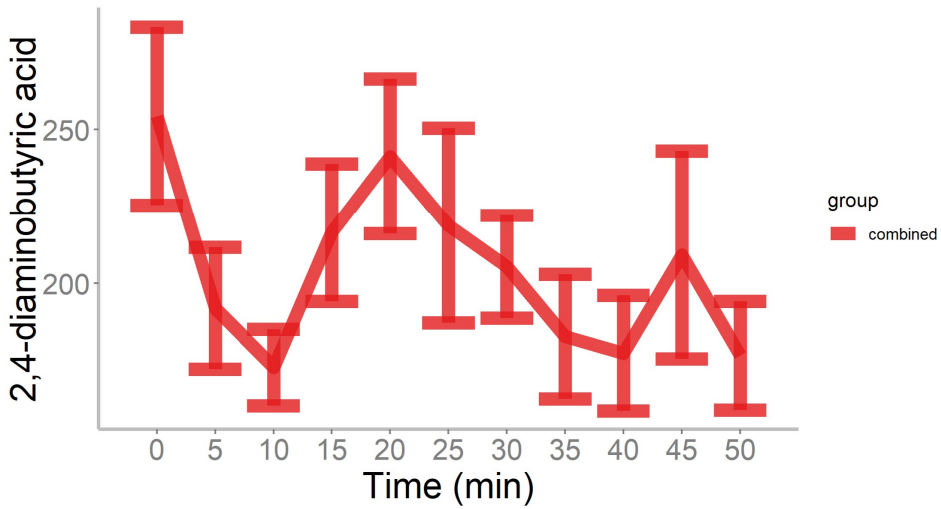

1,5-anhydroglucitol
40000
35000
30000
25000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

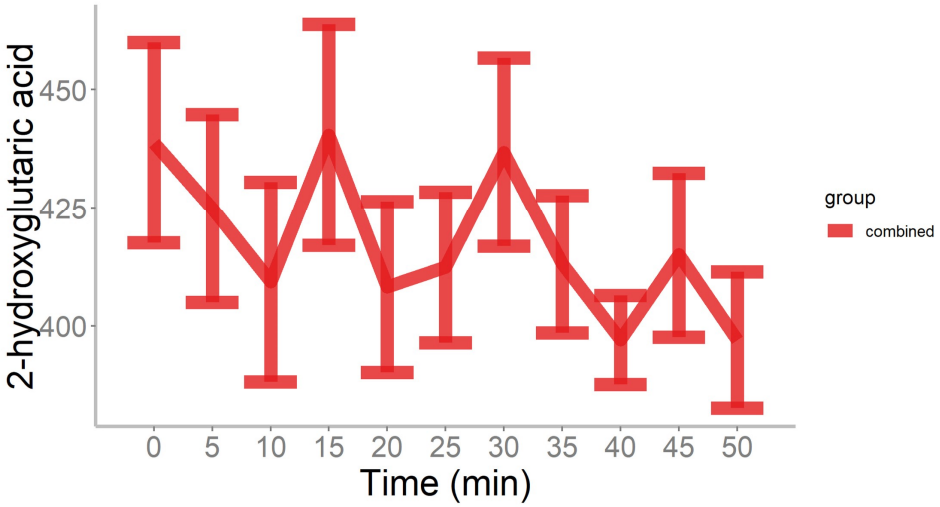

1-monopalmitin
350
300
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

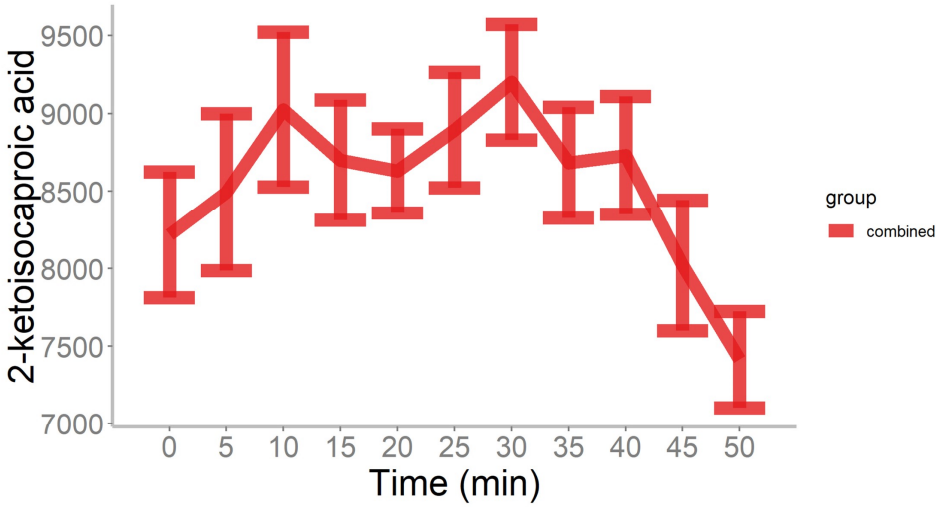

2,3-dihydroxybutanoic acid NIS
280
270
260
250
240
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

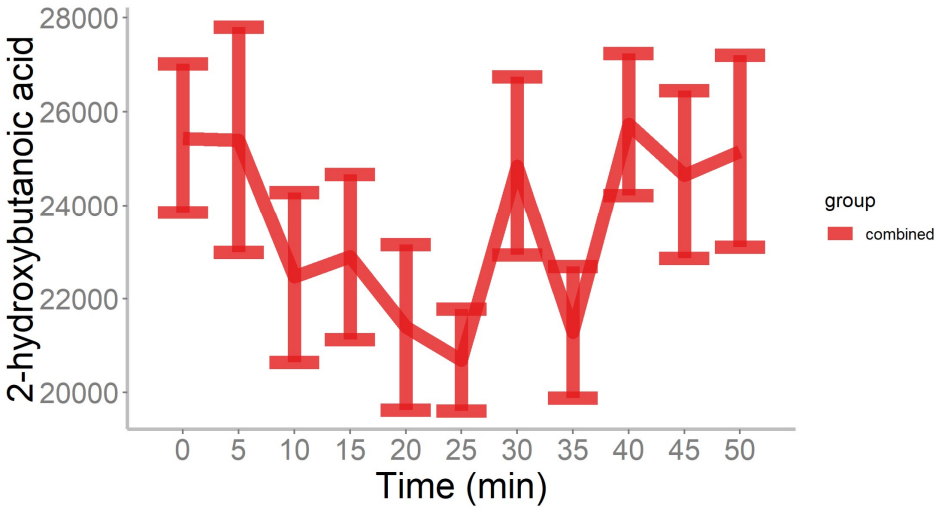

2-deoxytetronic acid NIST
1700
1600
1500
1400
1300
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

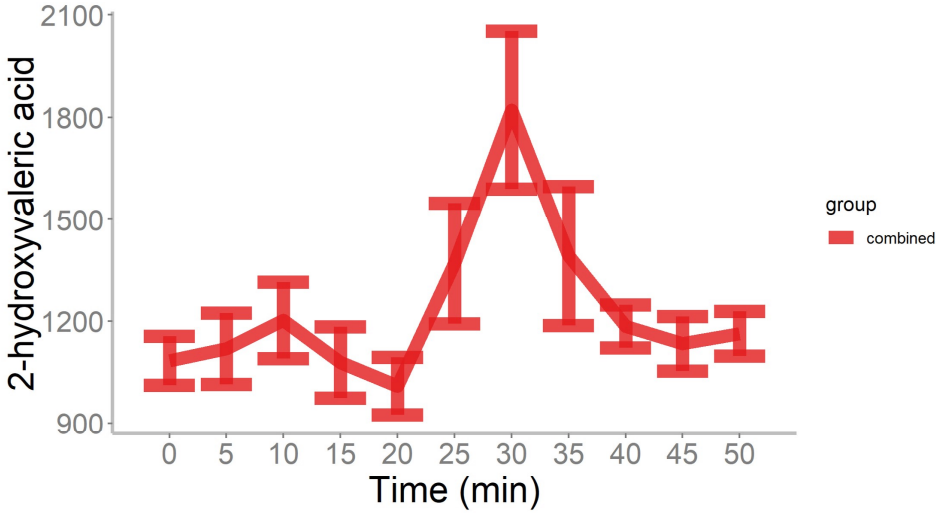

2,3,5-trihydroxypyrazine NIS
120
110
100
90
80
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

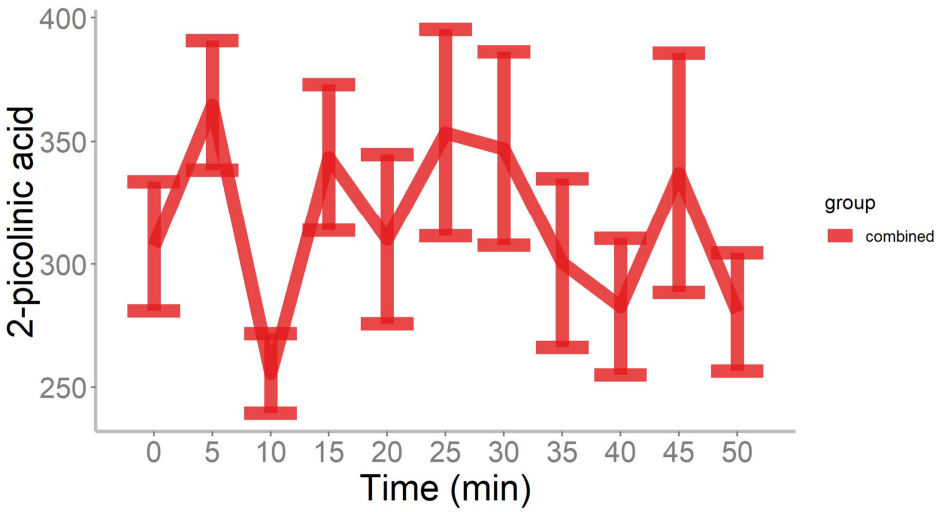

2,4-diaminobutyric acid
250
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

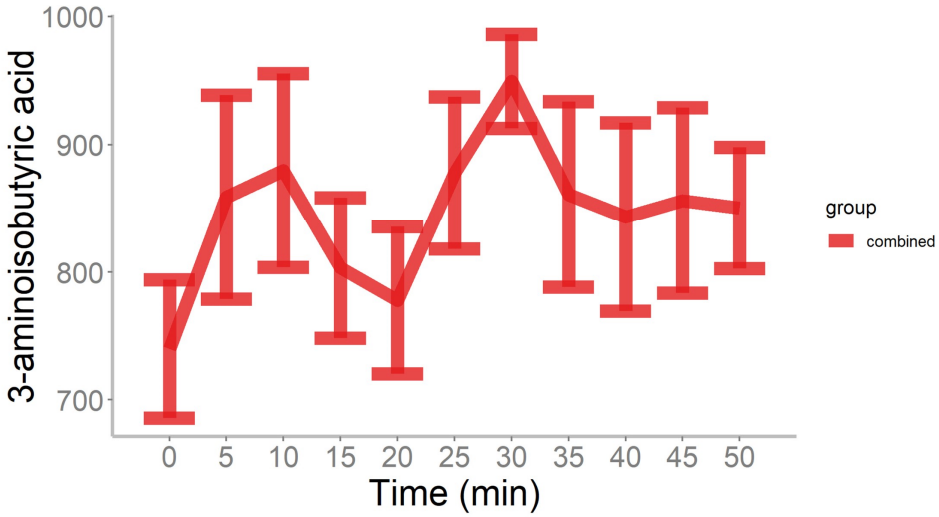

2-hydroxyglutaric acid
450
425
400
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

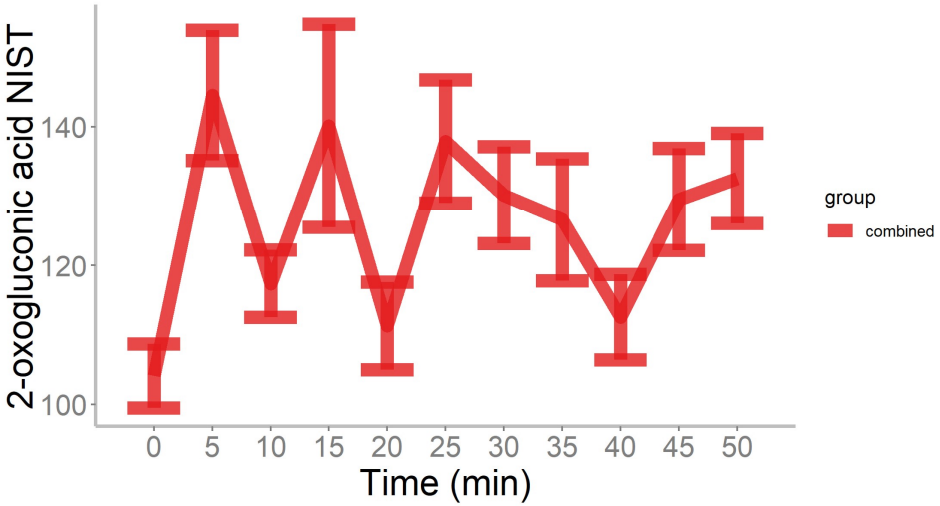

2-ketoisocaproic acid
9500
9000
8500
8000
7500
7000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

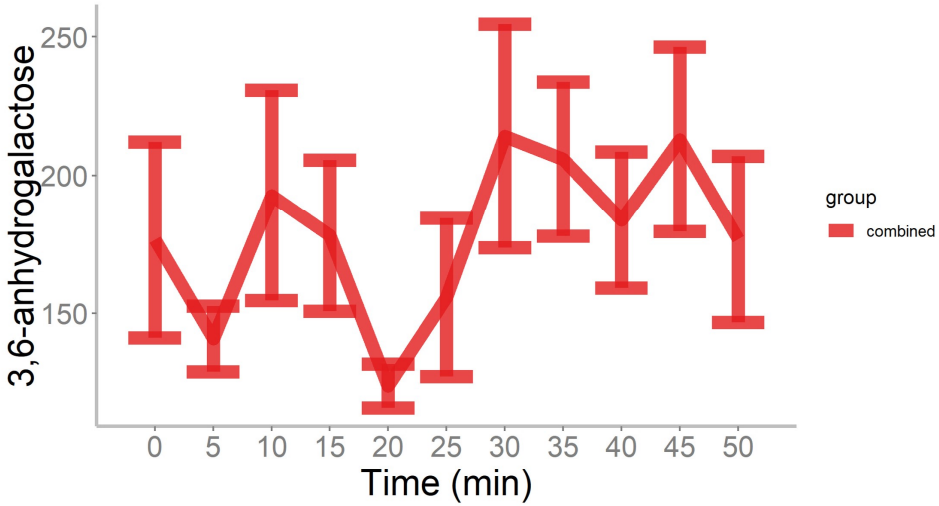

2-hydroxybutanoic acid
28000
26000
24000
22000
20000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

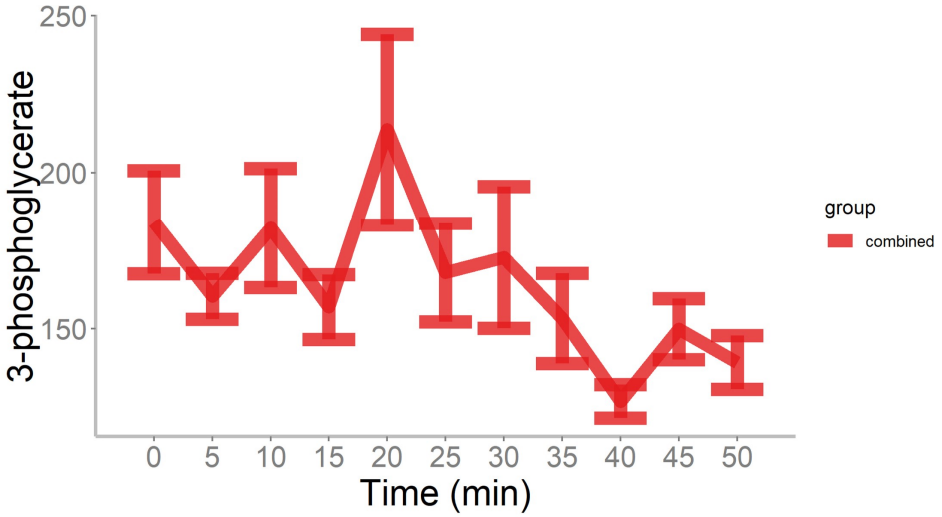

2-hydroxyvaleric acid
2100
1800
1500
1200
900
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

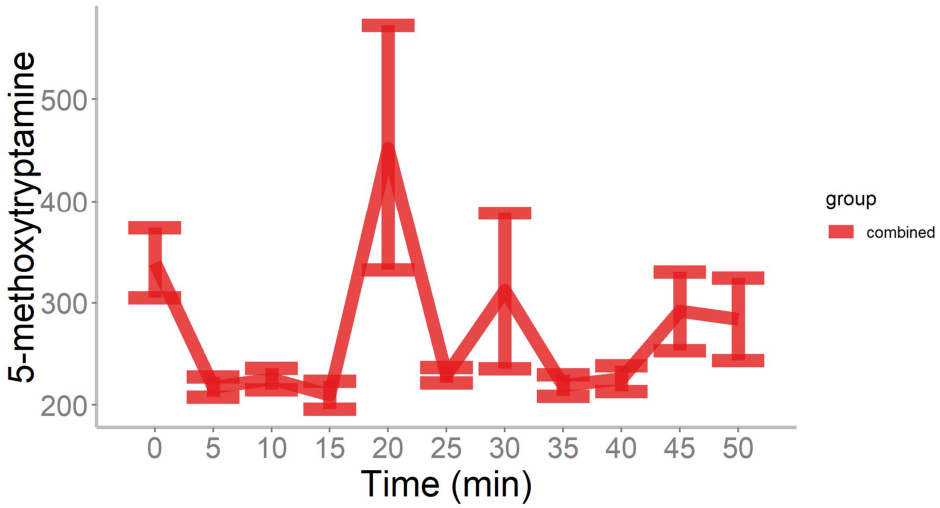

2-picolinic acid
400
350
300
250
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

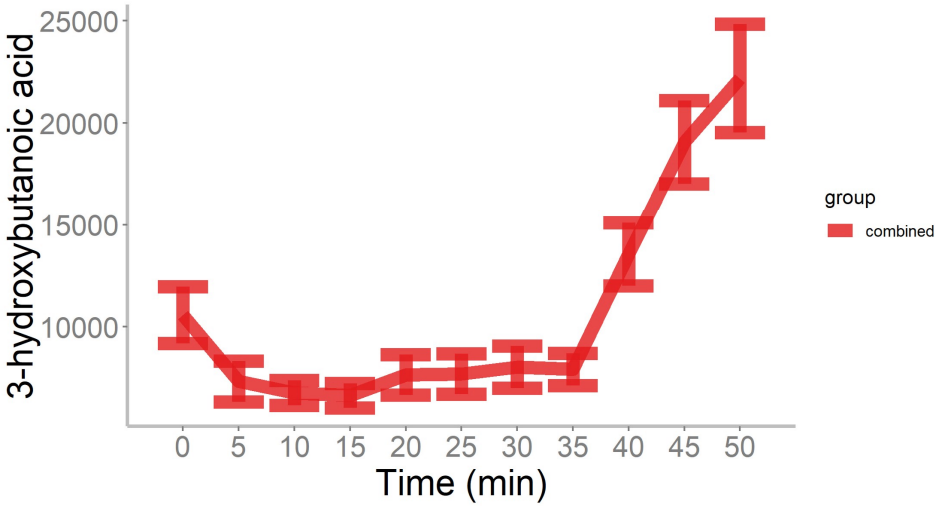

3-aminoisobutyric acid
1000
900
800
700
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

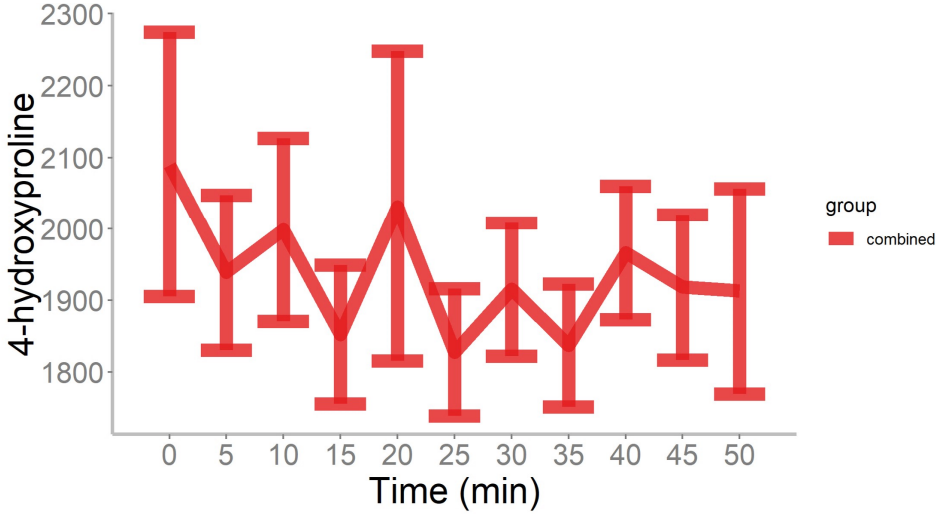

2-oxogluconic acid NIST
140
120
100
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined

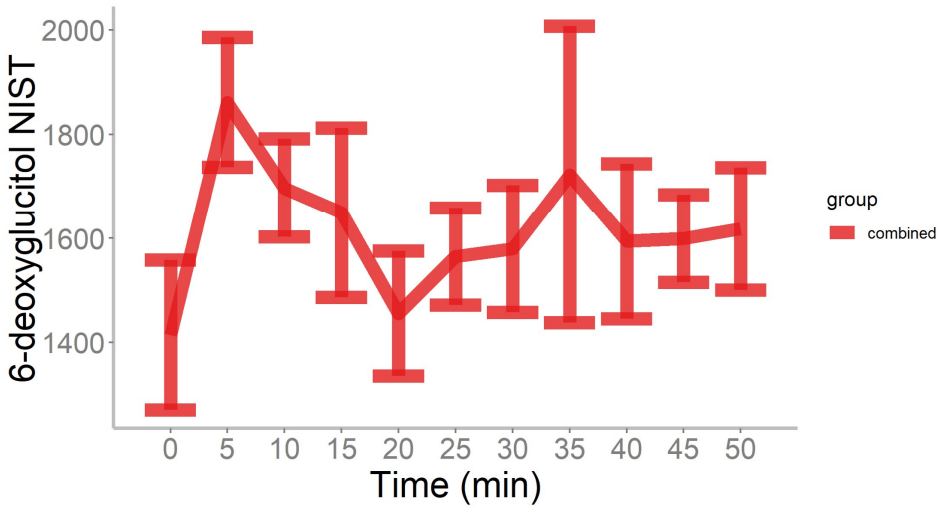

3,6-anhydrogalactose
250
200
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


3-phosphoglycerate
250
200
150
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


5-methoxytryptamine
500
400
300
200
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


3-hydroxybutanoic acid
25000
20000
15000
10000
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


4-hydroxyproline
2300
2200
2100
2000
1900
1800
0 5 10 15 20 25 30 35 40 45 50
Time (min)
group
combined


6-deoxyglucitol NIST
2000
1800
1600
1400
0
5
10
15
20
25
30
35
40
45
50
Time (min)
group
combined