

Supplementary tables and figures:

Table S1. ¹H NMR data and assignments of the metabolites in rat plasma.

Table S2. Significant changes in plasma metabolites at 6 h.

Table S3. Significant changes in plasma metabolites at 24 h.

Figure S1. Prediction tests for the models in Fig. 3.

Figure S2. Permutation test plots (200 permutations) for plasma at 6 h.

Figure S3. Permutation test plots (200 permutations) for plasma at 24 h.

Table S1. ¹H NMR data and assignments of the metabolites in rat plasma.

key	metabolites	$\delta^1\text{H}$ (ppm) ^a and multiplicity
1	lipids	0.89(m), 1.27(m)
2	isoleucine	0.94(t), 1.02(d)
3	leucine	0.95(d), 0.97(d)
4	valine	0.98(d), 1.04(d)
5	lactate	1.33(d), 4.11(q)
6	alanine	1.48(d)
7	acetate	1.92(s)
8	N-acetyl glycoprotein	2.04(s)
9	O-acetyl glycoprotein	2.14(s)
10	acetone	2.23(s)
11	acetoacetate	2.28(s)
12	pyruvate	2.38(s)
13	glutamine	2.44(m), 3.77(m), 2.15(m)
14	creatine	3.04(s), 3.93(s)
15	choline	3.19(s)
16	PC	3.23(s)
17	GPC	3.23(s)
18	taurine	3.25(t), 3.41(t)
19	TMAO	3.27(s)
20	betaine	3.27(s)
21	glycine	3.54(s)
22	glycerol	3.56(dd), 3.67(dd), 3.87(m)
23	α -glucose	5.24(d)
24	β -glucose	4.65(d)
25	unsaturated lipid	5.32(s)
26	tyrosine	6.88(d), 7.18(d)
27	1-methylhistidine	7.05(s), 7.75(s)
28	Phenylalanine	7.34(m), 7.38(m), 7.44(m)
29	formate	8.45(s)

^a Key: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; dd, doublet of doublet.

Table S2. Significant changes in plasma metabolites at 6 h.

key	Plasma metabolites	6 h Correlation coefficients (r^a)		
		model vs. control $R^2X=0.61$ $Q^2=0.89$	SA vs. model $R^2X=0.54$ $Q^2=0.61$	SA vs. control $R^2X=0.47$ $Q^2=0.51$
1	lactate	0.78	-0.73	0.64
2	alanine	0.71	-	0.63
3	acetone	0.73	-0.74	-
4	acetoacetate	0.66	-	0.64
5	acetate	0.72	-0.73	-
6	creatine	0.69	-0.64	-
7	TMAO, betaine	-0.63	0.63	-
8	glycine	-0.65	0.64	-
9	glycerol	0.67	-	0.65

^a Correlation coefficients, positive and negative signs indicate positive and negative correlation in the concentrations, respectively. $P= 0.05$, $[r] = 0.63$ was used as the corresponding cutoff value of correlation coefficient for the statistical significance based on the discrimination significance, respectively. “-” means the correlation coefficient $[r]$ is less than the cutoff value.

Table S3. Significant changes in plasma metabolites at 24 h.

key	Plasma metabolites	24 h Correlation coefficients (r^a)		
		model vs. control $R^2X=0.56$ $Q^2=0.89$	SA vs. model $R^2X=0.65$ $Q^2=0.83$	SA vs. control $R^2X=0.62$ $Q^2=0.75$
1	lactate	0.64	-0.66	-
2	TMAO, betaine	-0.64	0.64	-
3	glycine	-0.63	0.63	-
4	glycerol	0.72	-0.72	-

^a Correlation coefficients, positive and negative signs indicate positive and negative correlation in the concentrations, respectively. $P= 0.05$, $[r] = 0.63$ was used as the corresponding cutoff value of correlation coefficient for the statistical significance based on the discrimination significance, respectively. “-” means the correlation coefficient $[r]$ is less than the cutoff value.

Figure S1. Prediction tests for the models in Fig. 3.

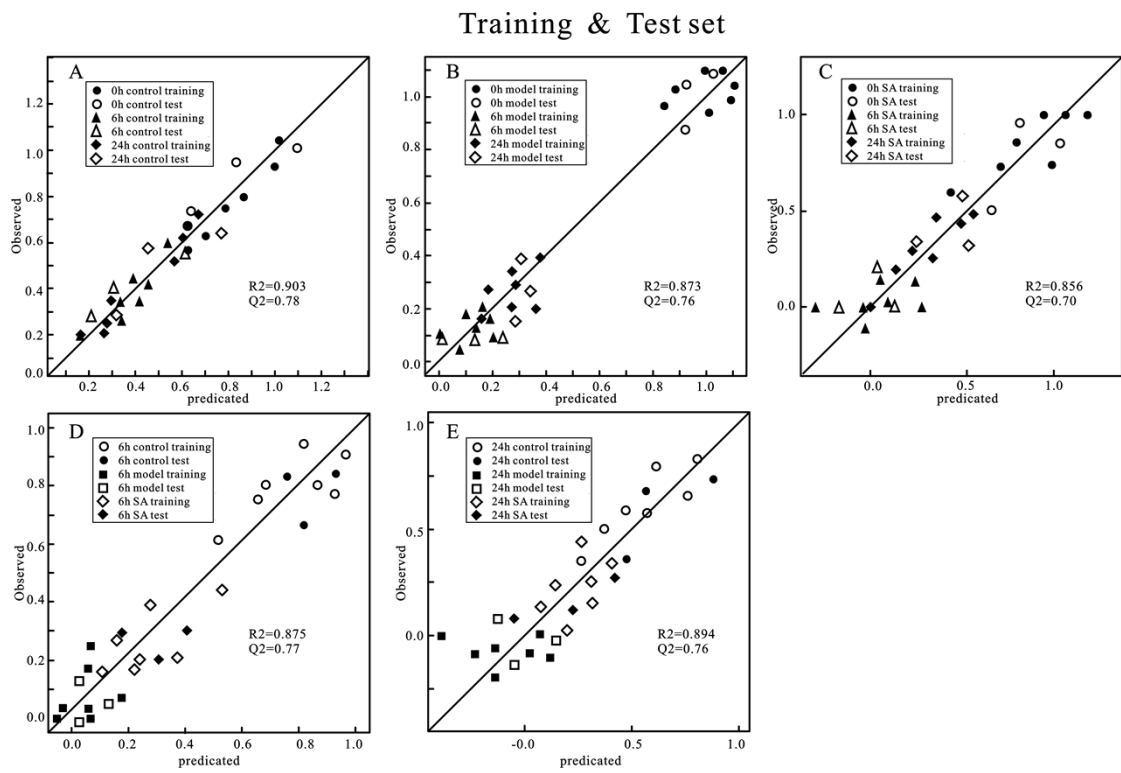


Figure S2. Permutation test plots (200 permutations) for plasma at 6 h. a1: model vs control, a2: SA vs model, a3: SA vs control.

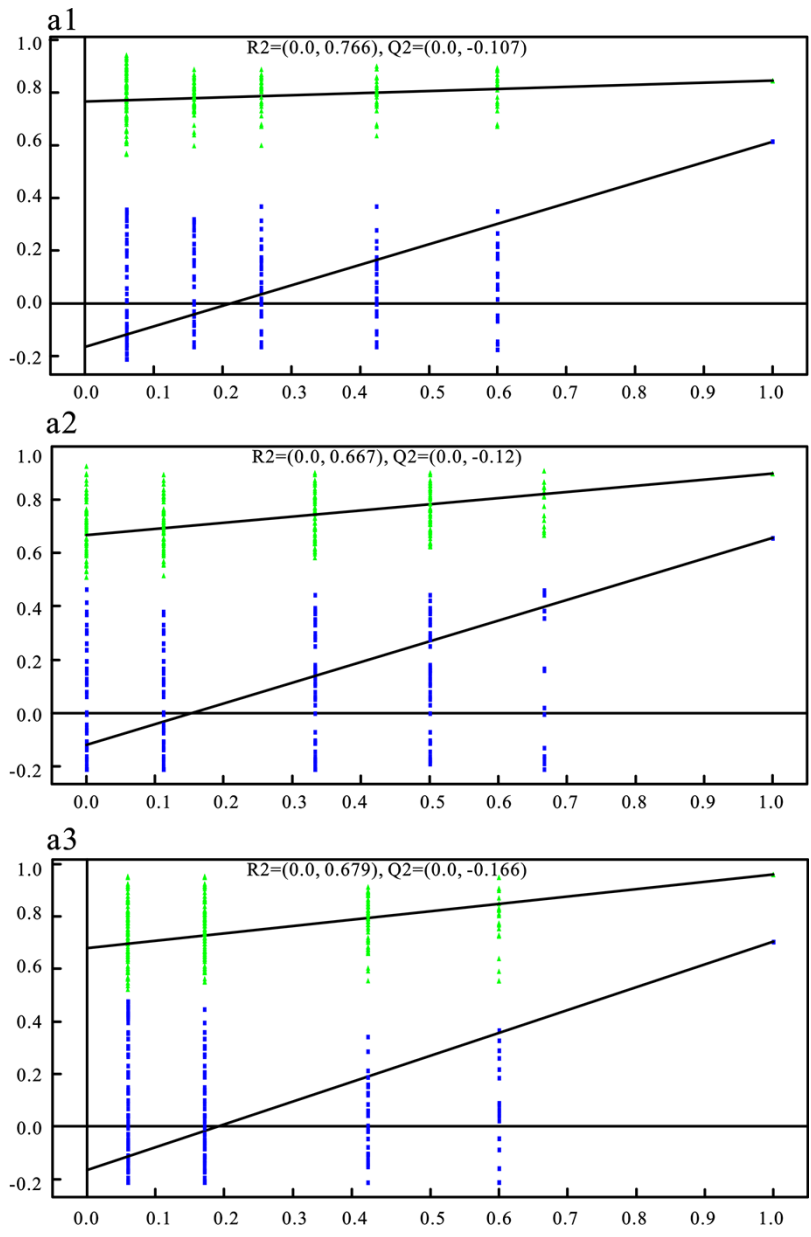


Figure S3. Permutation test plots (200 permutations) for plasma at 24 h. a1: model vs control, a2: SA vs model, a3: SA vs control.

