Supplementary Materials: Optimized Method for Untargeted Metabolomics Analysis of MDA-MB-231 Breast Cancer Cells

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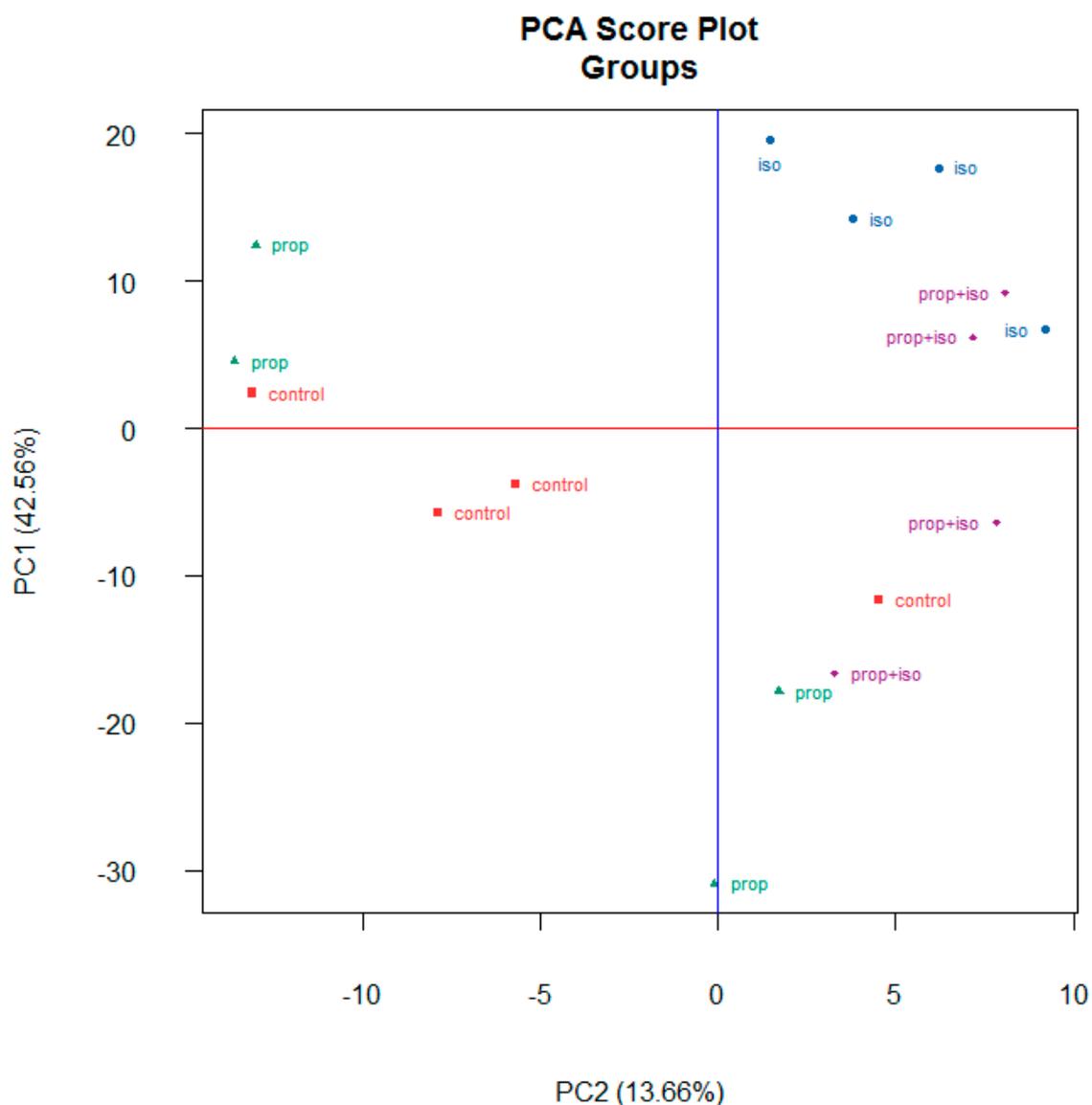**Figure S1.** Principal components analysis scores plot for the first two principal components from untargeted metabolomics analysis of MDA-MB-231 cells treated for 4 h with isoproterenol (Iso), propranolol (Prop), combination of isoproterenol and propranolol (Prop + Iso) or untreated control cells (control). Values in parenthesis indicate the percentage of variance explained by each principal component.

Table S1. Carbon-13 isotope enrichment of metabolites in cultured MDA-MB-231 cells following incubation with 50% U-^{13}C-glucose.

Metabolite	%Carbons Labelled																		
	Total	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
D-Glucose $C_6H_{12}O_6$	52%	44%	3%	0%	0%	0%	1%	52%											
D-Glucose 6-phosphate $C_6H_{13}O_9P$	50%	46%	3%	0%	3%	0%	1%	46%											
D-Fructose 6-phosphate $C_6H_{13}O_9P$	44%	53%	4%	0%	5%	0%	1%	37%											
D-Fructose 1,6-bisphosphate $C_6H_{14}O_{12}P_2$	61%	36%	3%	0%	21%	1%	2%	37%											
D-Glyceraldehyde 3-phosphate $C_3H_7O_6P$	36%	62%	2%	1%	36%														
Glycerone phosphate $C_3H_7O_6P$	50%	48%	2%	1%	48%														
3-Phospho-D-glycerate $C_3H_7O_7P$	49%	49%	2%	1%	48%														
Phosphoenolpyruvate $C_3H_5O_6P$	49%	49%	2%	3%	46%														
(*S*)-Lactate $C_3H_6O_3$	36%	62%	3%	1%	35%														
6-Phospho-D-gluconate $C_6H_{13}O_{10}P$	52%	45%	3%	0%	7%	0%	2%	42%											
D-Ribose 5-phosphate $C_5H_{11}O_8P$	71%	28%	3%	21%	22%	2%	25%												
Citrate $C_6H_8O_7$	38%	58%	5%	25%	8%	2%	3%	0%											
Isocitrate $C_6H_8O_7$	38%	58%	5%	25%	8%	2%	3%	0%											
2-Oxoglutarate $C_5H_6O_5$	9%	86%	5%	7%	1%	0%	0%												
D-Glutamate $C_5H_9NO_4$	9%	86%	5%	7%	1%	0%	0%												
(*S*)-Malate $C_4H_6O_5$	15%	81%	4%	4%	10%	0%													
L-Aspartate $C_4H_7NO_4$	14%	82%	4%	4%	10%	0%													
UDP-*N*-acetyl-D-glucosamine $C_{17}H_{27}N_3O_{17}P_2$	27%	61%	13%	7%	3%	1%	2%	9%	1%	3%	0%	0%	0%	0%	0%	0%	0%	0%	0%
GDP-L-fucose $C_{16}H_{25}N_5O_{15}P_2$	29%	59%	12%	5%	5%	0%	3%	15%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	
UDP-glucose $C_{15}H_{24}N_2O_{17}P_2$	67%	28%	5%	2%	5%	1%	2%	48%	6%	1%	1%	0%	0%	0%	0%	0%			
UDP-D-xylose $C_{14}H_{22}N_2O_{16}P_2$	18%	71%	10%	2%	0%	0%	16%	0%	0%	0%	0%	0%	0%	0%	0%				
UDP-glucuronate $C_{15}H_{22}N_2O_{18}P_2$	42%	49%	9%	3%	4%	1%	1%	28%	3%	1%	0%	0%	0%	0%	0%	0%			
ATP $C_{10}H_{16}N_5O_{13}P_3$	16%	75%	10%	6%	4%	1%	5%	0%	0%	0%	0%								
ADP $C_{10}H_{15}N_5O_{10}P_2$	8%	82%	9%	3%	3%	0%	3%	0%	0%	0%	0%								
Inosine $C_{10}H_{12}N_4O_5$	54%	41%	4%	16%	17%	0%	21%	0%	0%	0%	0%								
Guanosine $C_{10}H_{13}N_5O_5$	22%	70%	7%	7%	7%	0%	9%	0%	0%	0%	0%								
GTP $C_{10}H_{16}N_5O_{14}P_3$	28%	65%	9%	9%	7%	1%	9%	0%	0%	0%	0%								
O-Acetylcarnitine $C_9H_{17}NO_4$	25%	68%	7%	24%	2%	0%	0%	0%	0%	0%									
O-Butanoylcarnitine $C_{11}H_{21}NO_4$	42%	52%	7%	33%	3%	6%	0%	0%	0%	0%	0%	0%							
S-Adenosyl-L-methionine $C_{15}H_{22}N_6O_5S$	7%	79%	15%	0%	3%	0%	3%	0%	0%	0%	0%	0%	0%	0%	0%	0%			
Succinate $C_4H_6O_4$	3%	93%	5%	2%	0%	0%													

Table S2. Carbon-13 isotope enrichment of metabolites in cultured MDA-MB-231 cells following incubation with U-^{13}C-glutamine.

Metabolite	%Carbons Labelled																					
	Total	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
Citrate $C_6H_8O_7$	26%	69%	5%	2%	3%	17%	4%	0%														
2-Oxoglutarate $C_5H_6O_5$	46%	51%	3%	0%	3%	1%	42%															
L-Glutamate $C_5H_9NO_4$	46%	51%	3%	0%	3%	1%	41%															
(S)-Malate $C_4H_6O_5$	28%	69%	3%	0%	3%	25%																
L-Aspartate $C_4H_7NO_4$	27%	70%	3%	0%	3%	24%																
5-Oxoproline $C_5H_7NO_3$	30%	66%	4%	0%	0%	1%	29%															
L-Proline $C_5H_9NO_2$	21%	75%	4%	0%	1%	1%	19%															
L-1-Pyrroline-3-hydroxy-5-carboxylate $C_5H_7NO_3$	30%	66%	4%	0%	0%	1%	29%															
Glutathione disulfide $C_{20}H_{32}N_6O_{12}S_2$	7%	74%	19%	0%	0%	0%	5%	1%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%	0%
Glutathione $C_{10}H_{17}N_3O_6S$	4%	86%	10%	0%	0%	0%	3%	0%	0%	0%	0%	0%										
Succinate $C_4H_6O_4$	21%	75%	4%	1%	0%	19%																