

TARGETED ANALYSIS	microM								
Metabolite	Sensitive S				Resistant R				
	239S_272	239S_273_dx	239S_273sn	Average	239R_765	239R_768	239R_773	Average	Fold Change R vs S
lysoPC a C16:0	4.55	3.55	3.12	3.74	1.55	2.79	2.69	2.34	-1.59
lysoPC a C17:0	0.13	0.10	0.09	0.11	0.04	0.07	0.09	0.07	-1.59
PC ae C30:1	0.04	0.06	0.04	0.05	0.01	0.02	0.04	0.02	-1.94
Acetylnornithine	1.11	1.15	0.80	1.02	1.33	2.47	1.84	1.88	1.84
Putrescine	12.43	13.98	9.46	11.96	5.82	8.93	7.95	7.57	-1.58
Hydroxyproline	3.29	3.91	3.68	3.63	10.94	11.81	6.36	9.70	2.67
Lysine	41.27	33.20	32.83	35.77	50.85	115.00	50.23	72.03	2.01
Serine	47.57	51.07	42.20	46.94	26.75	31.30	21.93	26.66	-1.76
SM (OH) C16:1	0.08	0.12	0.08	0.09	0.02	0.04	0.07	0.04	-2.24
Valerylcarnitine	0.82	0.57	0.80	0.73	0.33	0.42	0.21	0.32	-2.27

UNTARGETED ANALYSIS	peak intensity										
Metabolite			Sensitive S				Resistant R				
	Aduct	Mw_mean	239_272	239_273_DX	239_273_SN	Average	239_765	239_768	239_773	Average	Fold Change R vs S
Pyruvate	M-H	87.0089	27194.73	28971.02	21595.23	25920.32	18393.31	13247.82	20913.07	17518.07	-1.48
Oxalacetic acid	M-H	112.9856	90978.80	90982.21	88475.51	90145.50	93600.73	94912.33	93922.21	94145.09	1.04
Fumarate	M-H	115.0036	26739.47	31083.41	22524.44	26782.44	16068.92	13600.10	20586.47	16751.83	-1.60
Taurine	M-H	124.0073	270453.40	215748.90	249176.07	245126.12	282715.43	329270.06	225412.34	279132.61	1.14
Malate	M-H	133.0141	75048.60	99263.50	71718.49	82010.20	38151.24	49497.82	60735.95	49461.67	-1.66
Oxoglutaric acid	M-H	145.0140	2338.25	2000.06	3481.99	2606.77	4412.93	8852.05	6297.46	6520.81	2.50
Glutamic acid	M-H	146.0457	27510.52	27125.60	26139.08	26925.07	41454.04	43592.29	31258.87	38768.40	1.44
N-Acetyl-L-aspartic acid	M-H	174.0407	87379.41	180810.07	127591.19	131926.89	63908.50	117497.14	136483.63	105963.09	-1.25
D-Glucurono-6,3-lactone	M-H	175.0253	590803.41	596476.10	466087.69	551122.40	386412.54	205610.91	422691.88	338238.44	-1.63
2-Isopropylmalic acid	M-H	175.0620	3826.49	18007.35	0.00	7277.95	0.00	0.00	1189.51	396.50	-18.36
N-Acetylglutamic acid	M-H	188.0562	2455.09	4146.32	3593.07	3398.16	6316.39	7610.15	9123.23	7683.26	2.26
Citric acid	M-H	191.0195	28437.22	48794.96	43898.11	40376.76	18245.62	29951.28	36450.48	28215.79	-1.43
Glutamic acid 5-phosphate	M-H	226.0119	2967.92	2376.35	4307.15	3217.14	6136.40	12343.64	8814.17	9098.07	2.83
Fructose 6-phosphate	M-H	241.0116	6983.33	5708.90	10056.97	7583.07	13609.37	32504.02	22672.04	22928.47	3.02
Palmitic acid	M-H	255.2329	130629.97	217812.30	177980.02	175474.10	108266.31	224881.71	269788.30	200978.77	1.15
Oleic acid	M-H	281.2480	5406.54	11896.40	9392.70	8898.55	10093.32	12158.24	26103.30	16118.29	1.81
Valine	M+H	118.0865	457096.01	540580.29	510492.32	502722.87	218438.13	223259.37	323260.69	254986.06	-1.97
Creatine	M+H	132.0769	432260.08	389198.20	406463.61	409307.30	318880.95	251069.52	328073.36	299341.28	-1.37
Spermidine	M+H	146.1651	286822.37	172516.04	236504.62	231947.67	189338.43	142080.15	165709.30	165709.29	-1.40
Spermine	M+H	203.2232	337359.87	242466.39	279307.71	286377.99	170576.98	143060.93	171606.85	161748.26	-1.77
Acetylcarnitine	M+H	204.1242	739855.88	703406.38	741415.50	728225.92	580122.94	582134.38	751178.00	637811.77	-1.14
Isovalerylcarnitine	M+H	246.1703	117739.99	86324.71	138803.80	114289.50	28270.76	24458.97	40901.46	31210.40	-3.66