Supporting Information

A nano Ultra-Performance Liquid Chromatography – High Resolution Mass Spectrometry

Approach for Global Metabolomic Profiling and Case Study on Drug-Resistant Multiple

Myeloma

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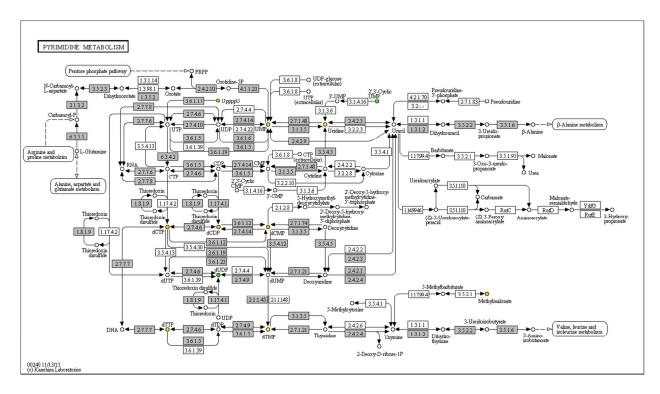


Figure S1. Example pathway enrichment analysis of regulated metabolites in BR and BS cell lines. Rectangular boxes represent gene products (e.g. enzymes) while circles represent metabolites. Various deoxy nucleotide phosphates show significant up(orange)/down(green) regulation including dCMP (34 Fold Change) and dUTP (-28 Fold Change).

	KEGG ID	Fold Change (BR/BS)
Porphyrin Metabolism		3 - (,
Protoporphyrinogen IX	C01079	32.4
Protoporphyrin	C02191	-12.9
Purine Metabolism		
ADP-ribose	C00301	13.6
SAICAR	C04823	3.7
Adenylosuccinate	C03794	-5.4
Guanosine monophosphate (GMP)	C00144	-3.3
Pyrimidine Metabolism		
Deoxycytidylic acid (dCMP)	C00239	34.0
2'-Deoxyuridine 5'-diphosphate (dUTP)	C01346	-28.2
Amino Sugar and Nucleotide Sugar Metabolism		
UDP-N-acetylglucosamine	C00043	7.0
CMP-N-glycolylneuraminate	C03691	10.0
Carbon Metabolism		
10-Formyl-THF	C00234	14.4
5,10-Methylene-THF	C00143	5.6
Tetrahydrofolate (THF)	C00101	10.6
Acetyl-CoA	C00024	16.3
Malonyl-CoA	C00083	12.9
Citramalyl-CoA	C01011	-86.5
Tetrahydrofolate (THF)	C00101	10.6

Table S1. Selected metabolite ontology enrichment of regulated metabolites identified in bortezomib resistant and sensitive myeloma cell lines. Data were generated with KegArray and show the fold-change between BR and BS cells. Negative values indicate down-regulation in BR cells as compared to BS cells.