

Supplementary Material: Development of an Optimized Protocol for NMR Metabolomics Studies of Human Colon Cancer Cell Lines and First Insight from Testing of the Protocol Using DNA G-Quadruplex Ligands as Novel Anti-Cancer Drugs

Ilaria Lauri, Francesco Savorani, Nunzia Iaccarino, Pasquale Zizza, Luigi Michele Pavone, Ettore Novellino, Søren Balling Engelsen and Antonio Randazzo

Probing the *Endo*-Metabolome of Human Colon Cancer Cell Lines by NMR Spectroscopy: Testing the Stimuli of DNA G-Quadruplex Ligands as Novel Anti-Cancer Drugs

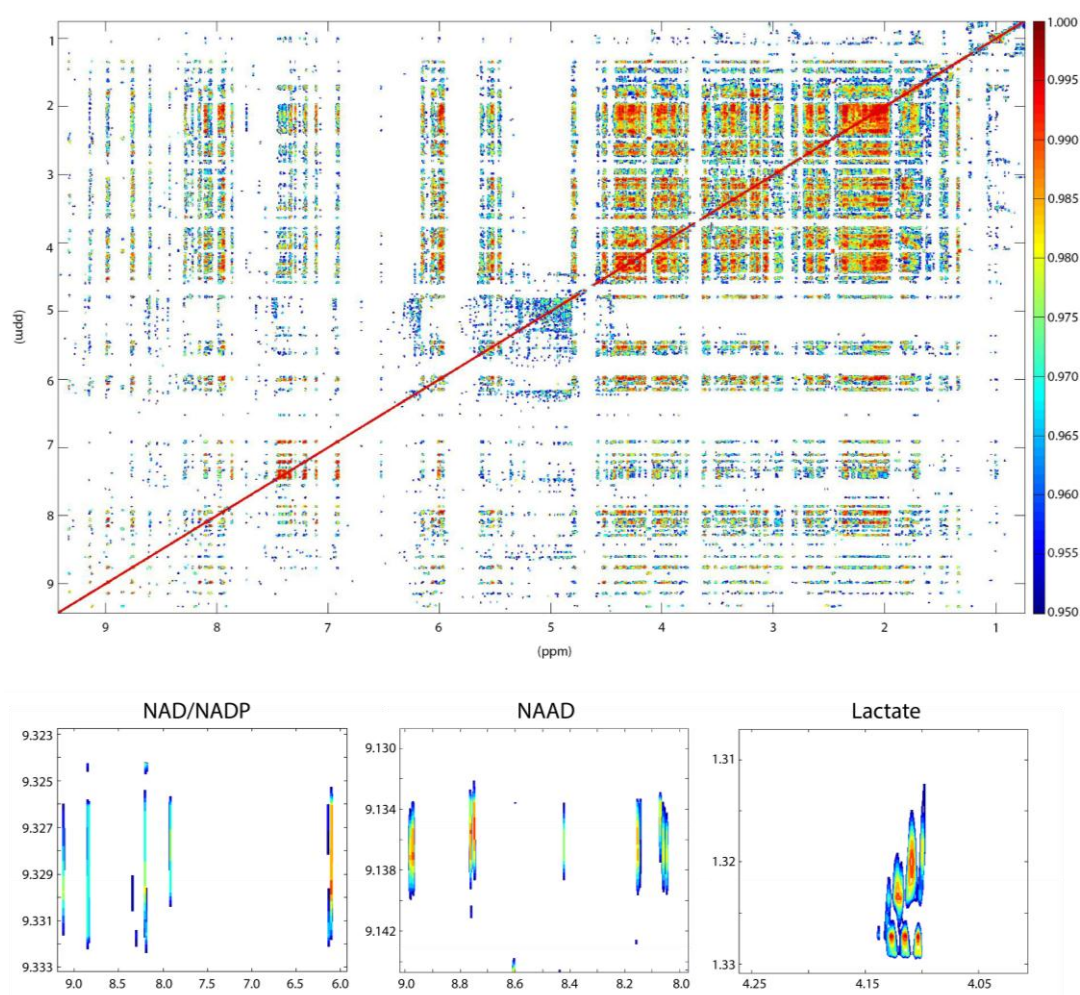


Figure S1. (A) Full STOCSY plot colored according to the correlation coefficient (see colored bar on the right); (B–D) Expanded regions of the STOCSY reporting the main correlations for NAD/NADP, NAAD and Lactate, respectively.

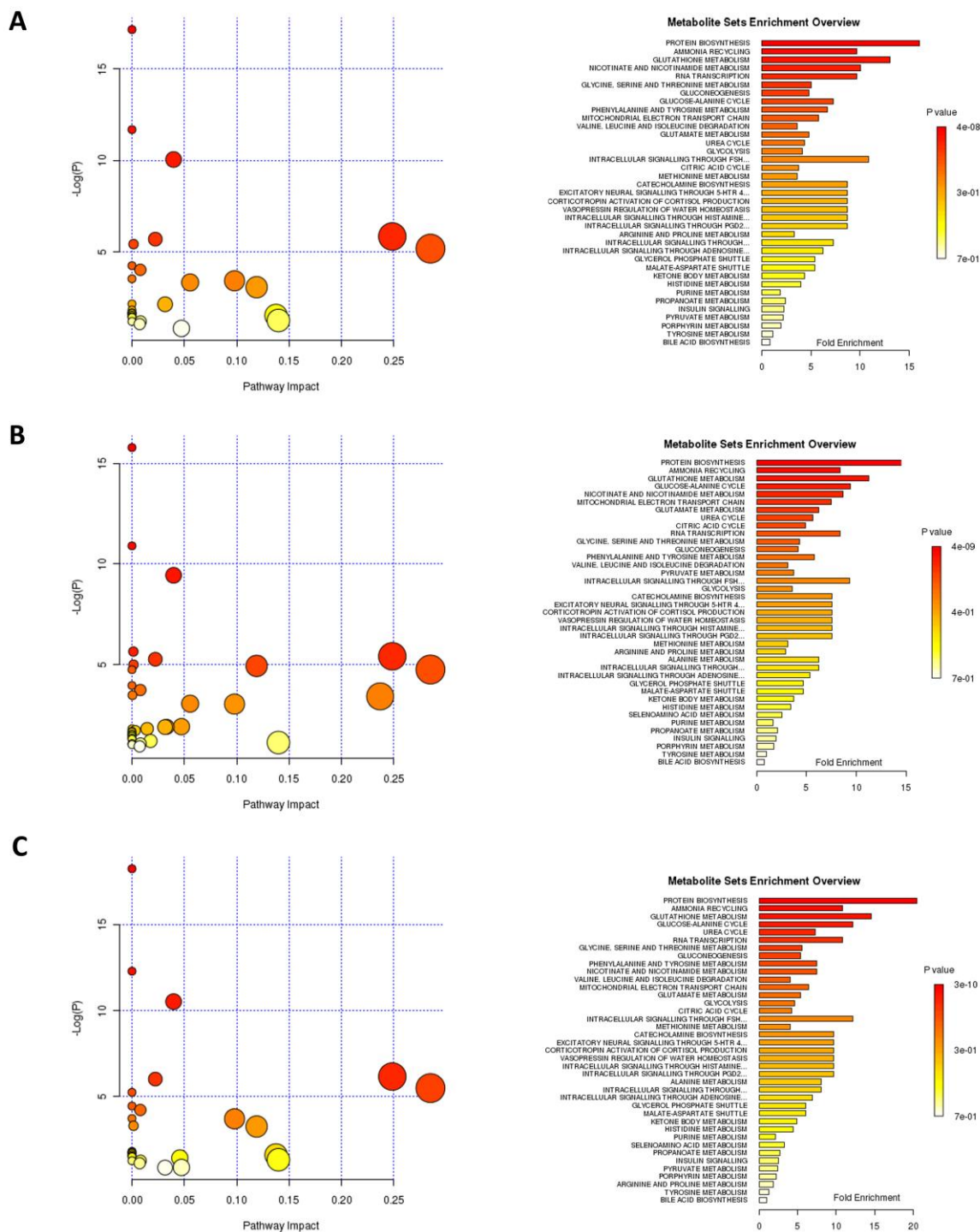


Figure S2. Impact of the treatment with compounds 1–3 (panel A–C, respectively) on metabolic pathways of HCT116 cell. Intracellular metabolite-based metabolic pathway analysis and metabolite sets enrichment overview are reported on the left and on the right, respectively.

Table S1. CHEBI codes for the identified metabolites.

Identification Number	Metabolite	CHEBI Code
1	Lactate	CHEBI:16651
2	Threonine	CHEBI:16857
3	Tyrosine	CHEBI:17895
4	Phenylalanine	CHEBI:17295
5	Creatine	CHEBI:16919
6	Creatine phosphate	CHEBI:17287
7	Glycine	CHEBI:15428
8	Alanine	CHEBI:16977
9	Acetate	CHEBI:30089
10	Succinate	CHEBI:30031
11	AMP	CHEBI:456215
		CHEBI:17191
12	Isoleucine, Leucine, Valine	CHEBI:15603
		CHEBI:16414
13	O-Phosphocholine	CHEBI:18132
14	Glycerophosphocholine	CHEBI:36313
15	Nicotinic acid adenine dinucleotide (NAAD)	CHEBI:75967
		CHEBI:57540
16	NAD ⁺ /NADP ⁺	CHEBI:58349
17	Histidine	CHEBI:15971
18	Glutathione	CHEBI:16856
19	ATP	CHEBI:30616