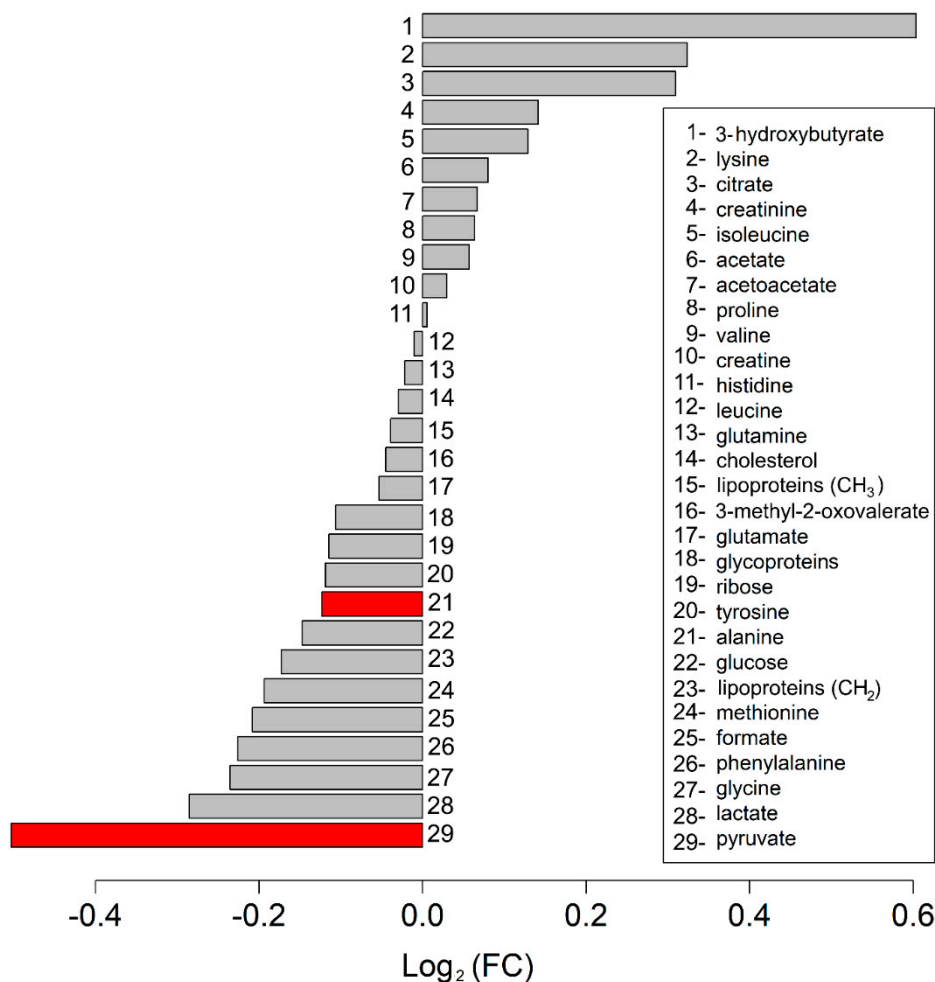


# Supplementary Materials: Metabolomics to Assess Response to Immune Checkpoint Inhibitors in Patients with Non-Small-Cell Lung Cancer

Veronica Ghini, Letizia Laera, Beatrice Fantechi, Francesca del Monte, Matteo Benelli, Amelia McCartney, Tenori Leonardo, Claudio Luchinat and Daniele Pozzessere



**Figure S1.** Bar plot reporting the values of Log<sub>2</sub> (Fold Change, FC) of quantified metabolites. Metabolites with Log<sub>2</sub> (FC) positive values have higher concentration in plasma samples from responder patients with respect to non-responders. Metabolites with Log<sub>2</sub> (FC) negative values have lower concentration in plasma samples from responder patients with respect to non-responders. Red bars represent *p*-values < 0.05.

**Table S1.** Patient and tumor characteristics for NSCLC cohort. NOS: not otherwise specified; SqCC: squamous histology; adeno: adenocarcinoma.

ID	Gender	Age	Histology	Site of Metastasis	Smoking Status	Drug
MetL01	F	60	NOS	lung, lymph nodes, adrenal, bone	Former	Niv
MetL05	M	69	SqCC	lung, trachea	Former	Niv
MetL06	M	69	SqCC	adrenal, colon	Current	Niv
MetL07	M	56	SqCC	lung, lymph nodes	Former	Niv
MetL09	M	45	SqCC	lung, bone, kidney	Current	Niv
MetL10	M	71	SqCC	lung, pleura	Former	Niv
MetL11	M	68	adeno	lung, lymph nodes	Current	Niv
MetL12	M	57	SqCC	lung, lymph nodes, bone, liver	Current	Niv
MetL13	F	75	adeno	lung, lymph nodes	Former	Niv
MetL15	F	73	adeno	lung, pleura	NA	Niv
MetL17	F	77	SqCC	lung	Former	Niv
MetL19	M	67	adeno	lung	Former	Niv
MetL20	F	74	SqCC	lung, lymph nodes, liver	Former	Niv
MetL22	M	59	adeno	lung, lymph nodes, bone, pleura	Current	Pem
MetL23	F	51	adeno	lung, lymph nodes	Current	Pem
MetL24	M	69	adeno	lung, bone	Former	Niv
MetL25	M	62	adeno	lung, lymph nodes	Former	Pem
MetL26	F	63	adeno	lymph nodes, bone	Former	Niv
MetL27	F	74	adeno	lung, lymph nodes, adrenal, bone	Never	Pem
MetL28	M	76	adeno	lymph nodes	Current	Pem
MetL29	F	70	SqCC	lung, pleura, bone	Current	Niv
MetL30	F	59	SqCC	lung, lymph nodes	Former	Niv
MetL31	M	84	adeno	lymph nodes, pleura	Former	Pem
MetL32	F	70	SqCC	lung, lymph nodes, adrenal, brain	Former	Niv
MetL33	M	77	SqCC	lung, lymph nodes	Former	Niv
MetL35	F	69	adeno	lung, lymph nodes, brain	Former	Pem
MetL34	F	48	adeno	lung, pleura, lymph nodes	NA	Niv
MetL36	M	76	adeno	lung, ureter, thoracic wall	Former	Niv
MetL37	M	75	SqCC	lung, lymph nodes, adrenal	Former	Niv
MetL38	F	81	adeno	lung, lymph nodes	Former	Pem

MetL39	M	68	adeno	lung, lymph nodes	Former	Niv
MetL40	M	71	adeno	lymph nodes, lung	Former	Niv
MetL41	M	73	SqCC	lung, lymph nodes, pleura, adrenal	Former	Niv
MetL42	F	70	SqCC	lung, lymph nodes	Current	Niv
MetL43	F	54	adeno	lung, lymph nodes, pleura, adrenal, bone	Current	Pem
MetL44	F	62	adeno	lung, lymph nodes, liver	Current	Niv
MetL45	F	71	SqCC	lung, lymph nodes, pleura, thoracic wall	Former	Niv
MetL46	M	61	adeno	lung, lymph nodes, brain	Current	Pem
MetL47	M	50	adeno	lung, lymph nodes, brain	Current	Pem
MetL48	M	68	SqCC	lung, lymph nodes	Former	Niv
MetL49	M	69	NOS	lung, liver, lymph nodes	Former	Niv
MetL50	M	83	SqCC	lung, lymph nodes	Former	Niv
MetL51	F	61	adeno	lung, brain	Former	Pem
MetL52	F	55	adeno	lung, lymph nodes, brain, adrenal	Former	Niv
MetL53	M	70	SqCC	lung, brain, liver, lymph nodes	Former	Niv
MetL55	M	72	adeno	lung, pleura, lymph nodes, bone	Current	Pem
MetL56	F	69	adeno	lung, brain, lymph nodes	Former	Pem
MetL57	M	56	adeno	lung, bone	Current	Niv
MetL59	F	37	adeno	lung, pleura	Never	Pem
MetL60	M	75	adeno	lung, bone	Current	Pem
MetL63	M	57	NOS	lung, brain, lymph nodes, adrenal	Current	Pem
MetL65	M	72	adeno	lung, lymph nodes	Current	Pem
MetL66	F	68	adeno	lung, pleura	Never	Pem

**Table S2.** List of the metabolites assigned and analyzed in serum samples of NSCLC patients. The Human Metabolome Database (HMDB) compound ID of each metabolite is reported.

Metabolites	HMDB ID
3-hydroxybutyrate	HMDB00011
3-methyl-2-oxovalerate	HMDB00491
Acetate	HMDB00042
Acetoacetate	HMDB00060
L-alanine	HMDB00161
Citrate	HMDB00094
Creatine	HMDB00064
Creatinine	HMDB00562
Cholesterol (CH <sub>3</sub> )	HMDB00067
Formate	HMDB00142
L-glycine	HMDB00123
D-glucose	HMDB00122
L-glutamate	HMDB00148
L-glutamine	HMDB00641
Glycoproteins (N-Acetyl)	-
L-histidine	HMDB00177
L-isoleucine	HMDB00172
Lactate	HMDB00190
L-leucine	HMDB00687
Lipoproteins (CH <sub>2</sub> )	-
Lipoproteins (CH <sub>3</sub> )	-
L-lysine	HMDB00182
L-methionine	HMDB00696
L-phenylalanine	HMDB00159
Pyruvate	HMDB00243
L-proline	HMDB00162
D-ribose	HMDB00283
L-tyrosine	HMDB00158
L-valine	HMDB00883

**Publisher's Note:** MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.



© 2020 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (<http://creativecommons.org/licenses/by/4.0/>).