

Discovering Associations between Clinical Parameters and Ex-Haled Air Spectral Characteristics of COVID-19 Patients: Supplementary Materials

Table S1 Description of blood parameters used in the study.

Blood parameter	Definition, clinical significance
ALT (alanine transaminase)	Intracellular enzyme involved in protein metabolism. An intracellular enzyme involved in protein metabolism [85]
aTTP (activated partial thromboplastin time)	Characterization of the coagulation process according to the “internal mechanism” [86]
AST (aspartate transaminase)	The enzyme, which is produced intracellularly in all cells of the body, is responsible for amino acid metabolism [87]
CI (color Index)	The blood color index reflects the degree of saturation of the erythrocyte with hemoglobin (normally 97% of the total cell mass), which forms a strong bond with oxygen for its transportation to the tissues [88]
CREAT (creatinine)	Acid is involved in energy metabolism. Formed in muscle tissue, excreted by the kidneys [89]
ESR (Erythrocyte Sedimentation Rate)	A test for the presence of inflammatory reactions occurring in the body, during which erythrocytes stick together [55]
FG (fibrinogen)	A glycoprotein synthesized in the liver is activated by thrombin and converted into insoluble fibrin, the basis of a clot during blood clotting. It is an indicator of hemostasis, [51] a primary marker of inflammation and necrosis [90]
GLU (glucose)	An organic compound that is a key metabolic substrate for energy production in tissues during glycolysis [40]
HGB (hemoglobin)	An iron-containing protein in red blood cells that can bind to oxygen molecules. 98% of oxygen is transported to tissues in the form of oxyhemoglobin [40]
INR (international normalized ratio)	Coefficient developed to standardize prothrombin time. It is the prothrombin ratio raised to the power of MIC (ISI, International Thromboplastin Reagent Sensitivity Index). It is a characteristic of the blood coagulation system [50]
LYM (lymphocytes)	A subgroup of leukocytes that carry out reactions of cellular and humoral immunity [42]
MONO (monocytes)	Large leukocytes of the system of mononuclear macrophages are part of all tissues. The main function is phagocytosis and intraplasmic digestion of foreign particles [43]
NEU (neutrophils)	The type of leukocytes, which are the first to arrive at the site of infection, secrete cytokines and chemokines that activate the inflammatory response, call for “reinforcement” in the form of other immune cells, launching an adaptive immune response [44]
PI (prothrombin index)	The ratio between the clotting time of the control plasma (“healthy”) and the patient sample (%) [91]
PLT (platelets)	Platelets formed in the bone marrow from megakaryocytes, the main function is to participate in blood coagulation in case of damage to the endothelial wall of the vessel [45]
PT (prothrombin time)	Parameter characterizing the duration of the blood coagulation process [38]
RBC (red blood cells)	Non-nuclear blood cells, biconcave disc shape. Functions of erythrocytes: transfer of oxygen to tissues; biosynthesis of glutathione; adsorption of amino acids, lipids, toxins; regulation of acid-base balance, etc. [92]

Table S1 Cont.

TBIL (total bilirubin)	The end product of heme metabolism, which is formed during the destruction of erythrocytes in tissues [88]
TP (total protein)	The total indicator of all protein fractions in the blood [88]
UREA (urea)	The main nitrogenous end product of protein and amino acid catabolism. Excreted from the body by the kidneys [74]
WBC (white blood cells)	A heterogeneous group of nucleated peripheral blood cells. Include: cells with cytoplasmic granulation/granularity - granulocytes (neutrophils, basophils and eosinophils) and without granularity - agranulocytes (lymphocytes and monocytes). They perform a protective function [42]

Table S2 Correlation coefficient values for pairwise distances distributions and Gaussian curve.

Group	Indicator/Parameter						
	ALT	aPTT	AST	CI	CREAT	ESR	FG
Healthy				0.950			
COVID-19 patient subgroups							
Below normal	–	0.949	–	0.954	–	0.982	0.970
Normal	0.983	0.977	0.984	0.984	0.991	0.988	0.995
Above normal	0.889	0.970	0.964	–	0.968	0.914	0.929
Subgroup	GLU	HGB	INR	LYM	MONO	NEU	PI
Below normal	–	0.979	–	0.976	–	0.979	0.981
Normal	0.985	0.991	0.991	0.991	0.985	0.983	–
Above normal	0.990	0.896	0.974	0.979	0.859	0.982	0.985
Subgroup	PLT	PT	RBC	TBIL	TP	UREA	WBC
Below normal	0.963	0.983	0.987	–	0.932	–	0.976
Normal	0.983	0.991	0.987	0.984	0.991	0.982	0.985
Above normal	–	0.919	–	0.845	–	0.957	–
Subgroup	D	HD	MD				
Presence	0.989	0.897	0.990				
Absence	0.974	0.959	0.956				
Subgroup	RF						
Absent	0.983						
I degree	0.980						
II degree	0.970						
Subgroup	Severity						
Mild	0.970						
Severe	0.980						

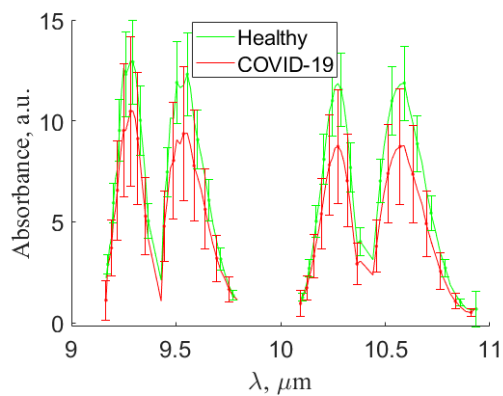


Fig. S1 The exhaled air IR absorption spectra of exhaled air from the COVID-19 patients and healthy participants presented in the terms of mean values and standard deviations.

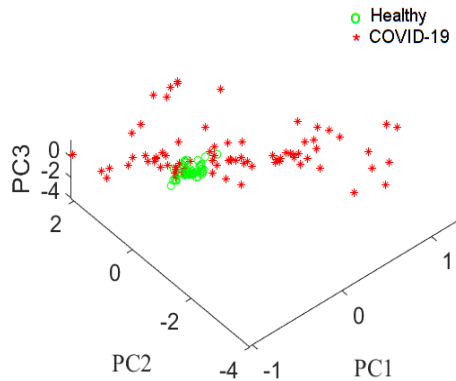


Fig. S2 Projections of the IR absorption spectra of exhaled air from COVID-19 patients and healthy participants in the space of the first, the second and the third principal components.