

Supplementary Information

Study of Organic Acids Profile in Human Urine by Capillary Zone Electrophoresis Aiming at the Diagnosis of COVID-19

Olívia B. O. Moreira,^a Luiz H. C. Adriano,^a Patrícia A. Geraldo,^a Pedro P. R. de Moura,^a Bruna M. Berlande,^a Fernanda A. Luna,^a Maria E. R. dos Santos,^a Raphaela C. C. Marques,^a Jéssica C. Q. de Souza,^a João M. B. Candido,^a Maria P. do Nascimento,^a Eliane B. T. de Lemos,^b Isabella S. B. Pinto,^b Lúcio M. de Lemos,^b Paula R. Chellini^{a,c} and Marcone A. L. de Oliveira,^{*,a,d}

^a*Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Juiz de Fora (UFJF), 36026-900 Juiz de Fora-MG, Brazil*

^b*Lemos Laboratório de Análises Clínicas, 36025-290 Juiz de Fora-MG, Brazil*

^c*Faculdade de Farmácia, Universidade Federal de Juiz de Fora (UFJF), 36026-900 Juiz de Fora-MG, Brazil*

^d*Instituto Nacional de Ciência e Tecnologia de Bioanalítica (INCTBio), Instituto de Química, Universidade de Campinas (UNICAMP), 13083-970 Campinas-SP, Brazil*

Olívia B. O. Moreira: <https://orcid.org/0000-0002-8073-4236>

Luiz H. C. Adriano: <https://orcid.org/0009-0008-3018-2737>

Patrícia A. Geraldo: <https://orcid.org/0000-0001-8692-6477>

Pedro P. R. de Moura: <https://orcid.org/0009-0006-1891-8145>

Bruna M. Berlande: <https://orcid.org/0009-0007-3376-2748>

Fernanda A. Luna: <https://orcid.org/0009-0007-7353-2621>

Maria E. R. dos Santos: <https://orcid.org/0009-0009-7953-7452>

Raphaela C. C. Marques: <https://orcid.org/0009-0004-3569-9576>

Jéssica C. Q. de Souza: <https://orcid.org/0000-0001-5278-9865>

João M. B. Candido: <https://orcid.org/0000-0002-6791-2624>

Maria P. do Nascimento: <https://orcid.org/0000-0002-6152-3644>

Paula R. Chellini: <https://orcid.org/0000-0001-8927-446X>

Marcone A. L. de Oliveira: <https://orcid.org/0000-0001-6026-9608>

*e-mail: marcone.oliveira@ufjf.br

Table S1. Complementary information about the volunteers in the study

COLLECTION DATE	ANALYSIS CODE	SEX	AGE	RT-PCR RESULT	BLOOD TYPE	RH FACTOR	PREVIOUS COVID DIAGNOSIS	VACCINE	ARTROTRAL DISEASES HISTORY	SMOKER	CHRONIC DISEASES	MEDICATIONS	SYMPTOMS
2021-09-21 00:00:00	1	Male	58	Negative	Not Determined	Not Determined	No	No	No	No	No	No	No
2021-08-13 00:00:00	2	Male	77	Negative	A	Not Determined	No	1st and 2nd doses - AstraZeneca	No	No	No	Rosuvastatin	No
2021-09-22 00:00:00	3	Female	39	Negative	O	Positive	No	1st and 2nd doses - Coronavac	No	No	No	No	No
2021-09-23 00:00:00	4	Male	37	Negative	A	Positive	No	1st and 2nd doses - PFIZER	No	No	No	No	No
2021-09-20 00:00:00	5	Female	37	Positive	O	Negative	No	1st and 2nd doses - AstraZeneca	No	No	No	No	No
2021-09-17 00:00:00	6	Female	22	Positive	A	Positive	No	1st dose - PFIZER	No	No	No	Purin F4	Persistent cough
2021-09-22 00:00:00	7	Male	51	Negative	O	Positive	No	1st dose - AstraZeneca	Dequie	No	No	No	Persistent cough, runny nose, headache
2021-09-20 00:00:00	8	Female	39	Positive	O	Positive	YES (13-04-2021)	1st dose - PFIZER	No	No	No	No	Runny nose, sore throat, inflamed throat
2021-09-22 00:00:00	9	Female	22	Negative	A	Negative	No	SDNOPHARM	Not Determined	No	No	No	Not Determined
2021-09-21 00:00:00	10	Male	53	Negative	O	Positive	No	1st and 2nd doses - AstraZeneca	Dequie	No	No	No	No
2021-09-11 00:00:00	11	Male	44	Negative	O	Positive	No	1st dose - AstraZeneca	No	No	No	No	No
2021-09-16 00:00:00	12	Female	65	Negative	O	Positive	No	1st and 2nd doses - AstraZeneca	No	No	Not Determined	Ivermectin	No
2021-09-15 00:00:00	13	Male	56	Positive	Not Determined	Not Determined	No	1st dose - AstraZeneca	No	No	No	No	Persistent cough, fever, body pain, headache
2021-09-13 00:00:00	14	Female	43	Positive	Not Determined	Not Determined	No	1st dose - AstraZeneca	Not Determined	No	No	No	Persistent cough, body pain, headache
2021-09-21 00:00:00	15	Female	41	Positive	A	Negative	No	Single dose - JANSSEN	No	No	No	Birth control pill	Fever
2021-07-19 00:00:00	16	Male	21	Negative	A	Positive	No	1st dose - AstraZeneca	Not Determined	No	No	No	Persistent cough, body pain, chest pain
2021-09-15 00:00:00	17	Female	65	Positive	A	Positive	No	1st and 2nd doses - Coronavac	Not Determined	No	No	No	Persistent cough, headache, malaise
2021-09-22 00:00:00	18	Female	41	Negative	O	Positive	YES (08-05-2021)	1st dose - PFIZER	Not Determined	Yes	No	No	Not Determined
2021-06-08 00:00:00	19	Female	55	Positive	B	Positive	No	1st dose - AstraZeneca	Dequie	No	Hypertension	No	Persistent cough, runny nose, headache, sore throat
2021-07-19 00:00:00	20	Female	59	Positive	A	Positive	YES (NOVEMBER/2021)	1st dose - AstraZeneca	No	No	No	No	Persistent cough, fever, headache
2021-07-26 00:00:00	21	Female	37	Negative	A	Positive	No	1st and 2nd doses - Coronavac	No	No	Ankylosing spondylitis	Nimesulide	Persistent cough, body pain, runny nose, headache
2021-07-22 00:00:00	22	Female	27	Negative	A	Positive	No	No	No	No	No	Desmoterol	No
2021-09-01 00:00:00	23	Female	38	Positive	A	Positive	No	1st dose - PFIZER	No	No	No	No	Persistent cough, fever, body pain, runny nose, headache
2021-09-22 00:00:00	24	Male	33	Positive	Not Determined	Not Determined	No	1st dose - AstraZeneca	No	No	No	No	No
2021-09-08 00:00:00	25	Female	37	Negative	B	Positive	No	1st and 2nd doses - AstraZeneca	Recurrent dengue	No	No	No	Persistent cough
2021-08-30 00:00:00	26	Male	33	Negative	A	Positive	YES (01-03-2021)	1st and 2nd doses - PFIZER	No	No	Diabetes	No	Body pain, headache, runny nose
2021-07-22 00:00:00	27	Male	27	Positive	A	Positive	No	No	No	No	No	No	Persistent cough, runny nose
2021-09-22 00:00:00	28	Female	44	Negative	B	Positive	No	1st and 2nd doses - Pfizer	No	No	No	No	No
2021-07-19 00:00:00	29	Female	41	Positive	Not Determined	Not Determined	No	1st and 2nd doses - Coronavac	No	No	No	No	Runny nose
2021-08-16 00:00:00	30	Female	36	Negative	O	Positive	No	1st dose - PFIZER	No	No	No	Ivermectin, bromazepam and paracetamol	Persistent cough, body pain, headache
2021-08-04 00:00:00	31	Female	29	Negative	O	Positive	No	1st dose - PFIZER	Not Determined	No	No	No	No
2021-08-21 00:00:00	32	Male	54	Negative	O	Negative	YES (24-07-2020)	1st and 2nd doses - AstraZeneca	Not Determined	No	Diabetes and hypertension	Salsob	Body pain, diarrhea, runny nose
2021-10-06 00:00:00	33	Male	34	Negative	A	Positive	No	1st and 2nd doses - AstraZeneca	Dequie	No	No	No	No
2021-09-15 00:00:00	34	Female	26	Positive	Not Determined	Not Determined	No	1st and 2nd doses - PFIZER	No	No	No	No	Persistent cough, runny nose, headache
2021-09-13 00:00:00	35	Male	29	Negative	O	Positive	No	1st dose - PFIZER	No	No	No	No	Persistent cough, diarrhea, runny nose, headache
2021-08-13 00:00:00	36	Female	50	Negative	O	Positive	No	1st and 2nd doses - Coronavac	Dequie	No	Sinusitis	Amphotericin	Persistent cough, body pain, runny nose
2021-09-02 00:00:00	37	Female	39	Positive	A	Positive	No	1st dose - PFIZER	No	No	No	No	Persistent cough, runny nose
2021-09-15 00:00:00	38	Male	27	Positive	Not Determined	Not Determined	No	1st dose - PFIZER	No	No	No	No	No
2021-09-13 00:00:00	39	Male	31	Positive	O	Positive	No	1st and 2nd doses - Coronavac	No	No	Hypertension	Eadolapil	No
2021-09-13 00:00:00	40	Male	35	Negative	Not Determined	Not Determined	No	1st dose - PFIZER	No	No	No	No	No
2021-09-13 00:00:00	41	Male	30	Negative	A	Positive	No	1st dose - AstraZeneca	No	No	No	No	Persistent cough, puck, diarrhea
2021-07-26 00:00:00	42	Male	53	Negative	O	Positive	YES (27-11-2020)	1st dose - AstraZeneca	No	No	No	No	No
2021-08-13 00:00:00	43	Male	39	Negative	A	Positive	No	1st dose - PFIZER	Not Determined	No	No	No	No
2021-09-13 00:00:00	44	Male	21	Positive	Not Determined	Not Determined	YES (15-03-2021)	1st and 2nd doses - AstraZeneca	No	No	No	No	No
2021-09-15 00:00:00	45	Male	39	Positive	O	Not Determined	No	1st and 2nd doses - Coronavac	Dequie	No	No	No	Body pain, runny nose
2021-09-16 00:00:00	46	Male	35	Negative	A	Positive	No	Single dose - JANSSEN	No	No	No	Corn and rocuronium	No
2021-09-14 00:00:00	47	Male	22	Negative	Not Determined	Not Determined	YES (JUNE/2020)	1st dose - PFIZER	Dequie	Yes	No	No	No
2021-07-26 00:00:00	48	Male	29	Positive	A	Positive	No	No	No	No	No	No	Persistent cough, fever, body pain, diarrhea, runny nose, headache
2021-09-08 00:00:00	49	Male	63	Positive	A	Positive	YES (20-11-2020)	Single dose - JANSSEN	No	No	Diabetes and heart problems	No	No
2021-09-08 00:00:00	50	Male	48	Negative	Not Determined	Not Determined	No	Not Determined	No	No	No	No	No
2021-09-23 00:00:00	51	Female	72	Negative	Not Determined	Not Determined	Yes	1st and 2nd doses - Coronavac	Not Determined	Yes	Hypertension	Not Determined	Yes

2021-09-27 00:00:00	52	Female	62	Negative	A	Positive	No	1st and 2nd doses - AstraZeneca	No	No	No	Enalapril	No
2021-09-25 00:00:00	53	Female	55	Positive	AB	Positive	No	1st and 2nd doses - AstraZeneca	No	No	No	No	No
2021-08-20 00:00:00	54	Female	54	Negative	O	Positive	No	Yes	Not Determined	No	No	No	No
2021-09-09 00:00:00	55	Male	44	Negative	B	Positive	No	1st and 2nd doses - PFIZER	No	No	No	No	No
2021-09-08 00:00:00	56	Male	40	Positive	A	Negative	No	1st dose - AstraZeneca	Dengue	No	No	Antihistamine, prednisone, and Allegra D	Persistent cough, body pain, runny nose, headache, nausea and dizziness
2021-09-08 00:00:00	57	Female	35	Positive	B	Positive	No	1st and 2nd doses - AstraZeneca	No	SDM	Thyroid	T4 LIVRE	Body pain, runny nose, headache
2021-09-23 00:00:00	58	Female	43	Negative	O	Positive	No	Not Determined	Dengue	No	No	No	No
2021-06-08 00:00:00	59	Male	50	Positive	A	Positive	YES (DECEMBER/2020)	1st and 2nd doses - AstraZeneca	Dengue	No	Hypertension	No	Persistent cough, runny nose, sore throat
2021-08-18 00:00:00	60	Female	32	Positive	O	Negative	No	1st and 2nd doses - Coronavac	Not Determined	No	No	Vitamin for FIP, A45, demerolone, primorone, and predalione	No
2021-08-16 00:00:00	61	Male	39	Negative	A	Positive	No	1st dose - PFIZER	Not Determined	No	No	No	No
2021-08-05 00:00:00	62	Female	26	Negative	A	Positive	No	No	No	No	No	No	No
2021-07-23 00:00:00	63	Male	68	Positive	A	Positive	YES (20/07/2021)	1st and 2nd doses - Coronavac	No	No	No	No	Persistent cough, fever, body pain, runny nose
2021-08-16 00:00:00	64	Male	35	Negative	Not Determined	Not Determined	No	1st dose - PFIZER	Not Determined	No	No	No	Fever, body pain, headache
2021-07-24 00:00:00	65	Male	45	Negative	AB	Positive	No	1st and 2nd doses - Coronavac	Not Determined	No	No	No	Runny nose
2021-07-17 00:00:00	66	Male	41	Negative	O	Negative	YES (15/11/2020)	1st and 2nd doses - AstraZeneca	Dengue	No	No	No	Persistent cough, runny nose, headache, loss of smell
2021-08-19 00:00:00	67	Female	72	Positive	Not Determined	Not Determined	No	1st and 2nd doses - Coronavac	Not Determined	No	Hypertension	Antihistamine	Flu, sore throat, rhinitis
2021-08-31 00:00:00	68	Female	26	Negative	A	Positive	No	1st dose - PFIZER	No	No	No	No	Persistent cough, runny nose
2021-07-08 00:00:00	69	Male	38	Negative	O	Positive	No	1st dose - PFIZER	Chikungunya	No	No	No	Fever, body pain, headache
2021-08-04 00:00:00	70	Female	35	Negative	AB	Positive	No	1st and 2nd doses - Coronavac	No	No	No	No	Body pain, runny nose, headache
2021-07-23 00:00:00	71	Female	45	Positive	A	Negative	No	1st and 2nd doses - Coronavac	Dengue	No	Hypertension	Hypertension medication	Persistent cough, fever, body pain, runny nose, headache
2021-08-20 00:00:00	72	Male	52	Negative	A	Negative	No	1st and 2nd doses - PFIZER	No	No	Hypertension	Pravastatin	Body pain, headache
2021-08-25 00:00:00	73	Female	29	Negative	O	Positive	YES (19/10/2021)	1st dose - PFIZER	Not Determined	No	No	No	Persistent cough, runny nose, headache
2021-07-19 00:00:00	74	Female	46	Negative	A	Positive	No	1st dose - AstraZeneca	Dengue	No	Asthma	No	No
2021-09-22 00:00:00	75	Female	39	Positive	A	Positive	No	Single dose - JANSSEN	No	No	No	No	Persistent cough, runny nose
2021-07-08 00:00:00	76	Female	38	Positive	Not Determined	Not Determined	YES (NOVEMBER/2020)	1st dose - AstraZeneca	Dengue	No	No	No	Fever, body pain, diarrhea, runny nose, headache
2021-08-14 00:00:00	77	Female	31	Negative	O	Positive	No	1st and 2nd doses - AstraZeneca	Not Determined	No	No	No	Persistent cough, runny nose, headache, nasal congestion
2021-08-14 00:00:00	78	Male	58	Positive	O	Positive	No	1st and 2nd doses - AstraZeneca	Not Determined	No	Diabetes	Antihistamine	Persistent cough, body pain, runny nose, headache
2021-07-22 00:00:00	79	Female	41	Positive	A	Positive	No	1st and 2nd doses - Coronavac	No	No	No	No	Funny nose, headache
2021-10-05 00:00:00	80	Male	43	Negative	Not Determined	Not Determined	No	1st and 2nd doses - MODERNA	No	No	No	No	No
2021-08-16 00:00:00	81	Male	31	Negative	A	Positive	YES (20/10/2020)	1st dose - PFIZER	Not Determined	Yes	No	Devote	No
2021-07-29 00:00:00	82	Male	29	Negative	A	Positive	No	Single dose - JANSSEN	No	No	No	No	Persistent cough, runny nose, headache
2021-08-24 00:00:00	83	Male	36	Negative	O	Positive	No	1st dose - AstraZeneca	Not Determined	No	No	Antihistamine	Funny nose, headache
2021-07-31 00:00:00	84	Male	23	Negative	A	Positive	No	Single dose - JANSSEN	No	Yes	No	No	No
2021-10-01 00:00:00	85	Male	37	Negative	B	Positive	YES (04/03/2021)	1st dose - AstraZeneca	No	No	No	No	No
2021-08-17 00:00:00	86	Female	30	Negative	A	Positive	No	1st dose - Coronavac	No	No	Respiratory problems	No	Headache
2021-10-08 00:00:00	87	Male	51	Negative	A	Positive	No	Single dose - JANSSEN	Not Determined	No	No	No	Funny nose, nasal congestion
2021-08-16 00:00:00	88	Female	42	Negative	O	Positive	YES (01/2021)	1st dose - PFIZER	No	No	No	No	Persistent cough, body pain
2021-07-22 00:00:00	89	Male	58	Negative	B	Positive	No	1st dose - AstraZeneca	No	No	No	No	Persistent cough, runny nose
2021-08-30 00:00:00	90	Male	40	Positive	B	Positive	No	1st and 2nd doses - AstraZeneca	No	No	No	No	Body pain, loss of smell
2021-09-21 00:00:00	91	Female	27	Positive	Not Determined	Not Determined	YES (08/09/2021)	1st dose - AstraZeneca	Not Determined	No	No	No	Persistent cough, body pain
2021-09-22 00:00:00	92	Female	51	Positive	A	Positive	No	Single dose - JANSSEN	No	No	No	No	Persistent cough, fever, pain, diarrhea, runny nose
2021-09-17 00:00:00	93	Female	39	Negative	O	Positive	No	Single dose - JANSSEN	Dengue (3 times)	No	No	Femiane	No
2021-07-22 00:00:00	94	Male	51	Negative	O	Positive	YES (15/01/2021)	Yes	No	No	No	No	Persistent cough, body pain, runny nose, headache
2021-07-19 00:00:00	95	Male	42	Negative	Not Determined	Not Determined	No	1st dose - PFIZER	No	No	No	No	No
2021-09-21 00:00:00	96	Male	41	Negative	O	Positive	No	Single dose - JANSSEN	No	No	No	No	Funny nose
2021-09-17 00:00:00	97	Male	49	Negative	O	Positive	No	No	No	Yes	No	Ivermectin and hydroxychloroquine	Fever, body pain, headache
2021-09-21 00:00:00	98	Female	52	Negative	O	Positive	YES (14/06/2021)	1st dose - AstraZeneca	No	No	Labyrinthitis	No	No
2021-08-02 00:00:00	99	Male	33	Positive	O	Positive	YES (APRIL/2021)	1st dose - PFIZER	No	No	Respiratory problems	Clenil	Persistent cough
2021-08-19 00:00:00	100	Male	29	Positive	A	Negative	No	1st dose - AstraZeneca	Not Determined	No	No	No	Persistent cough, body pain, loss of smell

Table S2. Optimized hyperparameters for the tested classification models

Model	Key hyperparameters and their values
PLS-DA	number of components: 2
SIMCA	number of components: 3
DT	criterion: gini; max features: none; min samples split: 6
RF	number of estimators: 819; max. features: sqrt; min. samples split: 26; min. samples leaf: 8; bootstrap: true
BT	number of trees: 100
SGD	loss: modified_huber; penalty: l1; alpha: 0.0516; learning rate: optimal; Eta0: 0.000193; max. iter: 2671; tol: 0.00069; early stopping: true

PLS-DA: partial least squares discriminant analysis; SIMCA: soft independent modeling of class analogy; DT: decision tree; RF: random forest; BT: bagged trees; SGD: stochastic gradient descent; max.: maximum; min.: minimum; iter: iterations; tol: tolerance.

