Effect of the 2020 lockdown during Covid-19 pandemic on the biomarkers of exposure to urban pollutants and oxidative stress in Rome residents

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Supplementary Table S1. Descriptive statistic of 28 urinary elements (μg/g creatinine) on 29 pairs of matched samples

Elements			year 2020					year 2021					
	LOD[a]	LOQ[b]	mean	SD[c]	median	min	max	mean	SD[c]	median	min	max	p-value[d]
As	2	8	122	289	36	4	1524	54	73	23	2	311	ns
B	30	120	**1650**	**910**	1390	377	4220	**2150**	**1500**	1740	736	8060	*
Ba	3	9	4.9	3.3	3.7	0.6	13.2	4.9	4.7	3.7	0.5	25.1	ns
Be	0.02	0.08	<0.02	-	<0.02	<0.02	<0.02	<0.02	-	<0.02	<0.02	<0.02	nd
Bi	0.01	0.03	0.02	0.05	0.01	<0.01	0.25	<0.01	-	<0.01	<0.01	0.03	ns
Ca	500	2000	198000	120000	172000	36086	504000	175000	120000	147000	29300	582000	ns
Cd	0.04	0.1	0.22	0.16	0.20	<0.04	0.69	0.24	0.16	0.20	<0.04	0.70	ns
Co	0.05	0.2	**0.56**	**0.45**	0.37	0.09	1.85	**0.87**	**0.57**	0.79	0.12	2.90	*
Cr	0.2	0.6	5.2	3.5	4.1	1.0	15.6	5.7	4.6	4.2	1.2	24.5	ns
Cs	0.01	0.03	19	21	13	3	94	25	29	14	4	105	ns
Cu	0.4	1	**30**	**18**	24	8	90	**40**	**27**	29	16	119	*
Fe	1	4	18	12	13	3	48	18.6	8.5	16	7	38	ns
Hg	0.03	0.09	0.62	0.41	0.49	0.13	1.71	0.69	0.48	0.51	0.14	2.14	ns
K	700	2500	1320000	830000	1010000	158000	3780000	1580000	900000	1310000	348000	4400000	ns
Li	0.04	0.1	27	37	13	3	182	22	19	14	3	71	ns
Mg	5	20	92820	43900	81100	37900	225000	90600	45200	83200	35300	241000	ns
Mn	5	20	<5	-	<5	<5	<5	<5	-	<5	<5	<5	nd
Mo	0.6	2	53	44	39	11	178	44	34	38	7	148	ns
Na	30	90	2550000	1900000	1860000	547000	950000	2460000	1700000	2080000	51700	8760000	ns
Ni	0.6	2	6.2	3.4	5.5	1.7	17.8	6.5	3.1	5.7	2.7	15.5	ns
Pb	0.04	0.1	1.2	1.1	0.8	0.2	4.4	1.0	0.5	1.0	0.3	2.3	ns
Rb	0.07	0.2	967	520	857	238	2050	1160	680	995	256	2740	ns
Sb	0.01	0.04	**6.9**	**5.1**	4.7	0.8	21.7	**8.9**	**5.7**	7.6	1.2	25.6	*

Se	1	3	34	16	33	15	79	33	16	29	16	76	ns
Sn	0.04	0.1	0.8	2.0	0.3	0.1	10.4	0.4	0.2	0.4	0.1	1.0	ns
Sr	0.5	2	199	100	168	59	538	195	120	184	40	619	ns
Te	0.2	0.5	15	33	5	0.4	179	13	16	7	2	76	ns
Tl	0.001	0.005	6.5	7.5	4.2	0.2	26.6	9.9	9.7	6.4	0.6	39.5	ns
V	0.3	1	1.6	2.4	0.3	0.3	9.0	0.9	1.5	0.3	0.3	6.5	ns
Zn	3	9	345	200	315	88	1160	394	200	323	91	791	ns

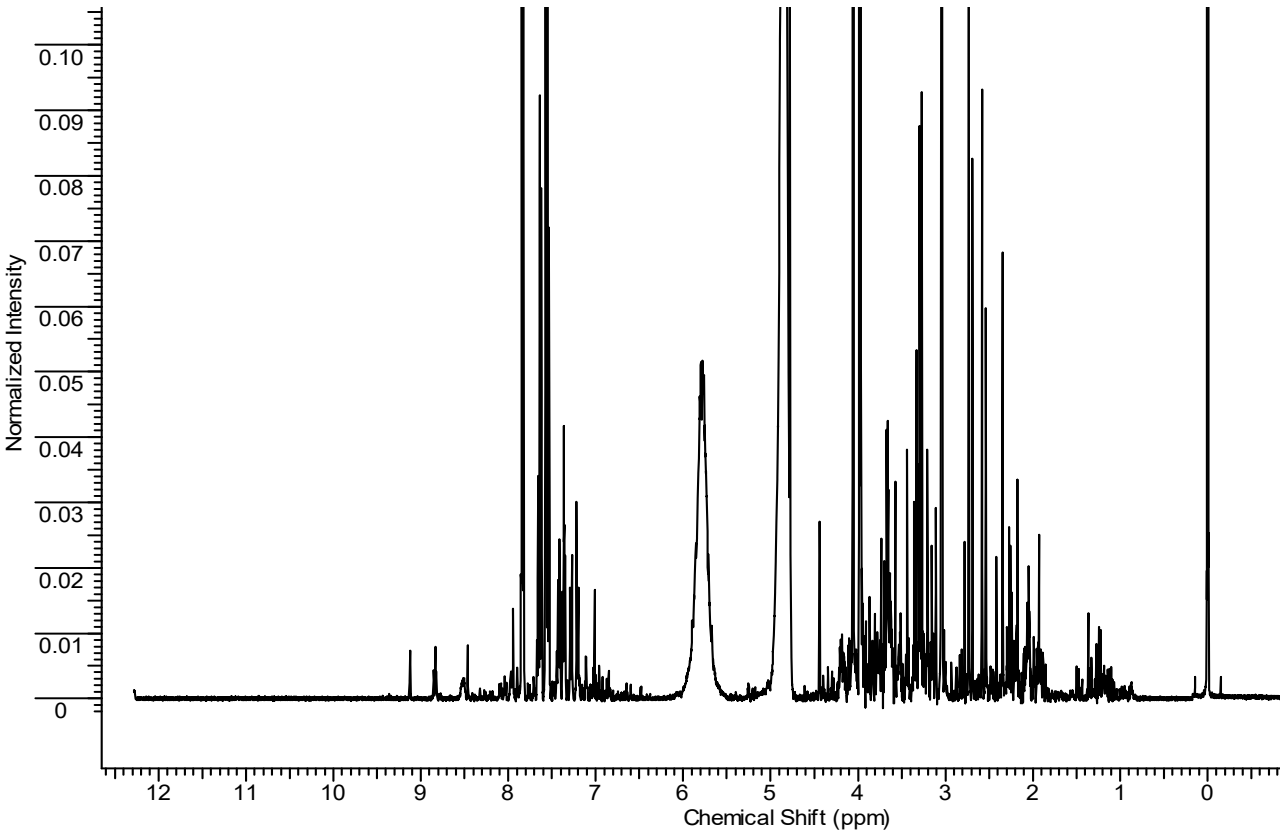
[a] LOD, limit of determination

[b] LOQ, limit of quantification

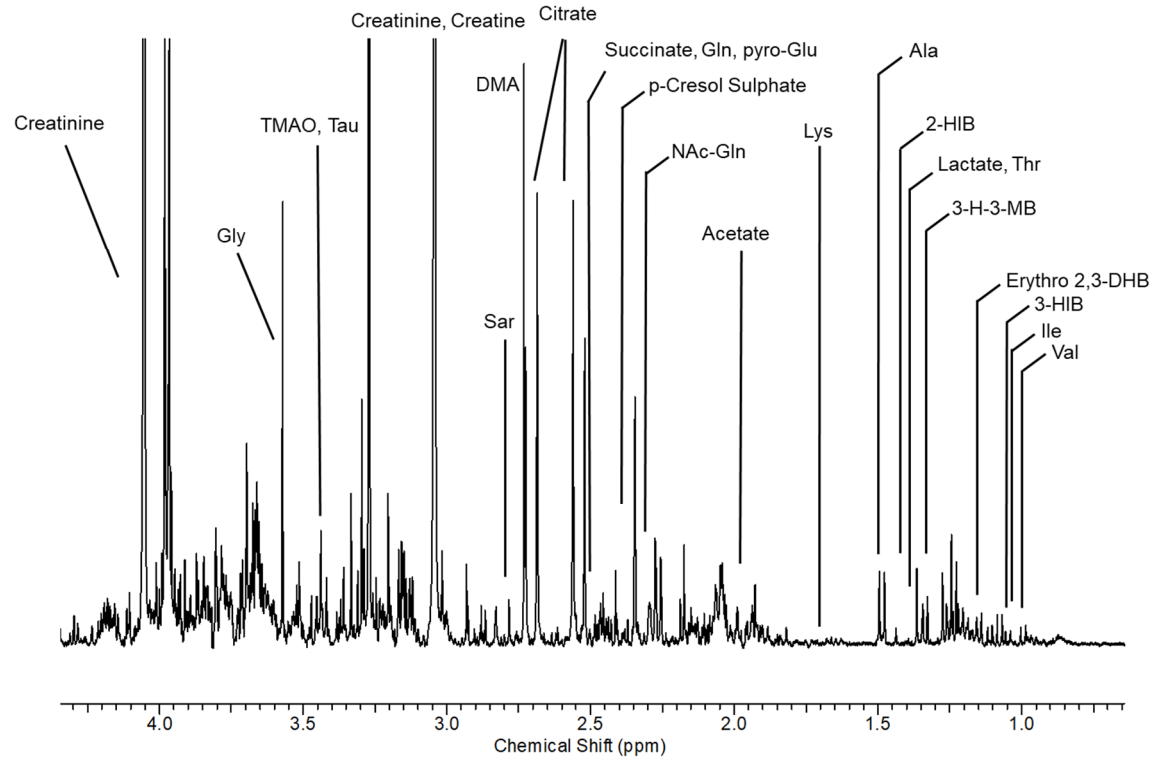
[c] SD, standard deviation

[d] Paired Student's t test was applied: "nd" = not determined; "ns" = not significant at $p > 0.05$; "*" = significant at $p < 0.05$. Numbers in bold in the same row indicate significant differences ($p < 0.05$).

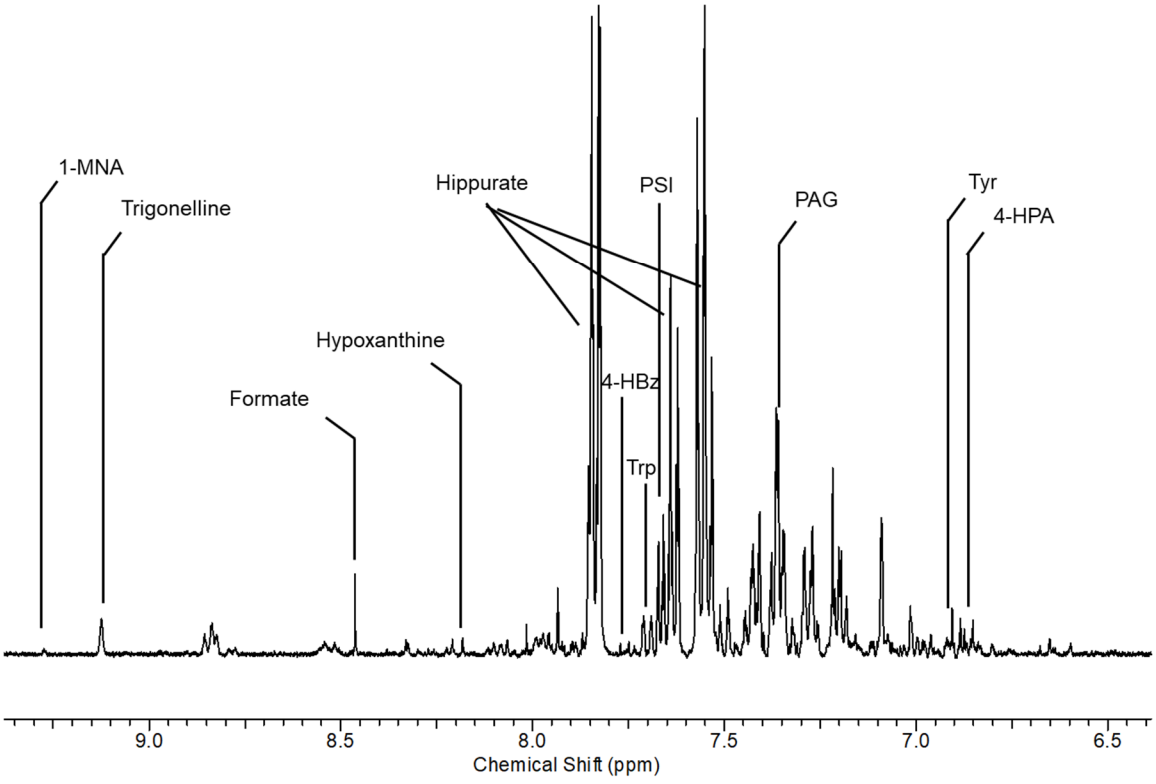
Supplementary Figure S1. ^{1}H NMR spectrum of urine



Supplementary Figure S2. ^{1}H NMR spectrum of urine, spectral region 1 – 4 ppm.

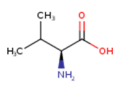
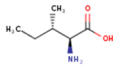
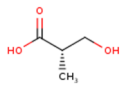
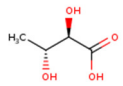
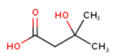
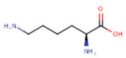
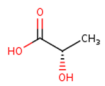
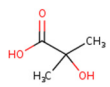
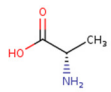
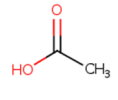


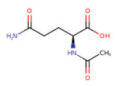
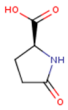
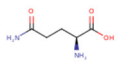
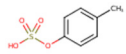
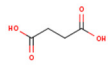
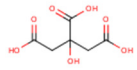
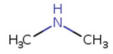
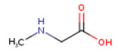
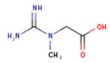
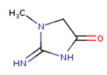
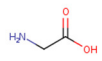
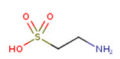
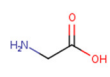
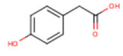
Supplementary Figure S3. ^{1}H NMR spectrum of urine, spectral region 6.5 – 9.5 ppm.

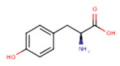
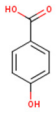
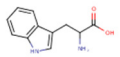
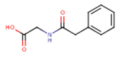
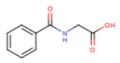
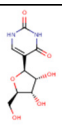
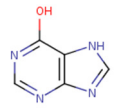
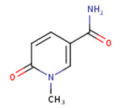
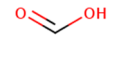
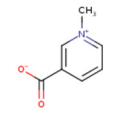
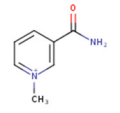


Supplementary Table S2. ^{1}H NMR assignment of urinary metabolites.

bs: broad singlet; d: doublet; dd: double doublet; m: multiplet; pd: pseudo doublet; q: quartet; s: singlet, t: triplet.

Metabolite	Structure	^{1}H δ ppm	Multiplicity	Assignment
1. Valine (Val)		0.99 **1.05**	d **d**	CH_3 **CH_3'**
2. Isoleucine (Ile)		0.92 **1.01** 1.99	t **d**	CH_3 **CH_3** CH
3. 3-Hydroxyisobutyrate (3-HIB)		**1.07** 2.49 3.54 3.71	**d**	**CH_3**
4. Erythro-2,3-dihydroxybutyrate (Erythro-2,3-DHB)		**1.11** 4.19	**d** m	**CH_3** CH
5. 3-Hydroxy-3-methylbutyrate (3-H-3-MB)		**1.27**	**s**	**CH_3, CH_3'**
6. Lysine (Lys)		1.48 **1.71** 1.89 3.02 3.74	m **m** m m m	CH_2 **CH_2** CH_2 CH_2 CH
7. Lactate		**1.33** 4.11	**d** q	**CH_3** CH
8. Threonine (Thr)		**1.33** 3.59 4.26	**d** d m	**CH_3** α-CH β-CH
9. 2-Hydroxyisobutyrate (2-HIB)		**1.36**	**s**	**CH_3, CH_3'**
10. Alanine (Ala)		**1.49** 3.78	**d** q	**CH_3** α-CH
11. Acetate		**1.93**	**s**	**CH_3**

12. N-acetylglutamine (NAcGln)		1.95 2.12 **2.27** 4.18 7.97	 **m** bs	 **CH_2**
13. Pyroglutamate (pyro-Glu)		2.03 **2.40** 2.50 4.19	m **m** m dd	CH_2 **CH** CH CH
14. Glutamine (Gln)		2.13 **2.46** 3.78	m **m** t	CH_2 **CH_2** CH
15. p-Cresol sulphate		**2.35** 7.21 7.28	**bs** dd dd	**CH_3** CH, CH′ CH, CH′
16. Succinate		**2.41**	**s**	**CH_2, CH_2′**
17. Citrate		**2.54** 2.69	**d** d	**CH, CH′** CH, CH′
18. Dimethylamine (DMA)		**2.73**	**s**	**CH_3, CH_3′**
19. Sarcosine (Sar)		**2.78**	**s**	**CH_3**
20. Creatine		**3.05** 3.95	**s** s	**CH_3** CH2
21. Creatinine		3.03 **4.05**	s **s**	CH_3 **CH_2**
22. Trimethylamine N-Oxide (TMAO)		**3.27**	**s**	**CH_3** CH_2
23. Taurine (Tau)		3.27 **3.43**	t **t**	CH_2 **CH_2**
24. Glycine (Gly)		**3.57**	**s**	**CH_2**
25. 4-Hydroxyphenylacetate (4-HPA)		**6.87** 7.17	**dd** dd	**CH,CH** CH,CH

26. Tyrosine (Tyr)		**6.90** 7.18	**dd** dd	**2-CH,6-CH** 3-CH,5-CH
27. 4-Hydroxybenzoate (4-HBz)		6.97 **7.76**	dd **dd**	2-CH,6-CH **3-CH,5-CH**
28. Tryptophan (Trp)		7.20 7.27- 7.29- **7.50** 7.70	- - - **pd** pd	3-CH 2-CH **5-CH** 4-CH
29. Phenylacetylglycine (PAG)		**7.36** 7.39 7.42	**m** m m	3,5-CH 4-CH 2,6-CH
30. Hippurate (Hipp)		3.97 **7.55** 7.64 7.83	d **m** m m	CH2 **3,5-CH** 4-CH 2,6-CH
31. Pseudouridine (PSI)		**7.67**	**bs**	**CH**
32. Hypoxanthine (HX)		**8.19** 8.21	s s	2-CH 7-CH
33. N1-Methyl-2-pyridone-5-carboxamide (2PY)		3.64 6.67 7.98 **8.33**	s d d **dd**	N-CH3 3-CH 4-CH **6-CH**
34. Formate		**8.46**	**s**	**CH**
35. U01		8.06 8.54 **8.78**	 **d**	 **6-CH**
36. Trigonelline (Trig)		4.44 8.08 8.84 **9.12**	s m m **s**	N-CH3 5-CH 4,6-CH **2-CH**
37. 1-MNA		8.17 8.89 8.96 **9.28**	t d d **s**	5-CH 4-CH 6-CH **2-CH**