

Supplementary Materials

A New Method for the Assessment of the Oxidative Potential of Both Water-Soluble and Insoluble PM

Maria Agostina Frezzini, Gianluca Di Iulio, Caterina Tiraboschi, Silvia Canepari and Lorenzo Massimi *

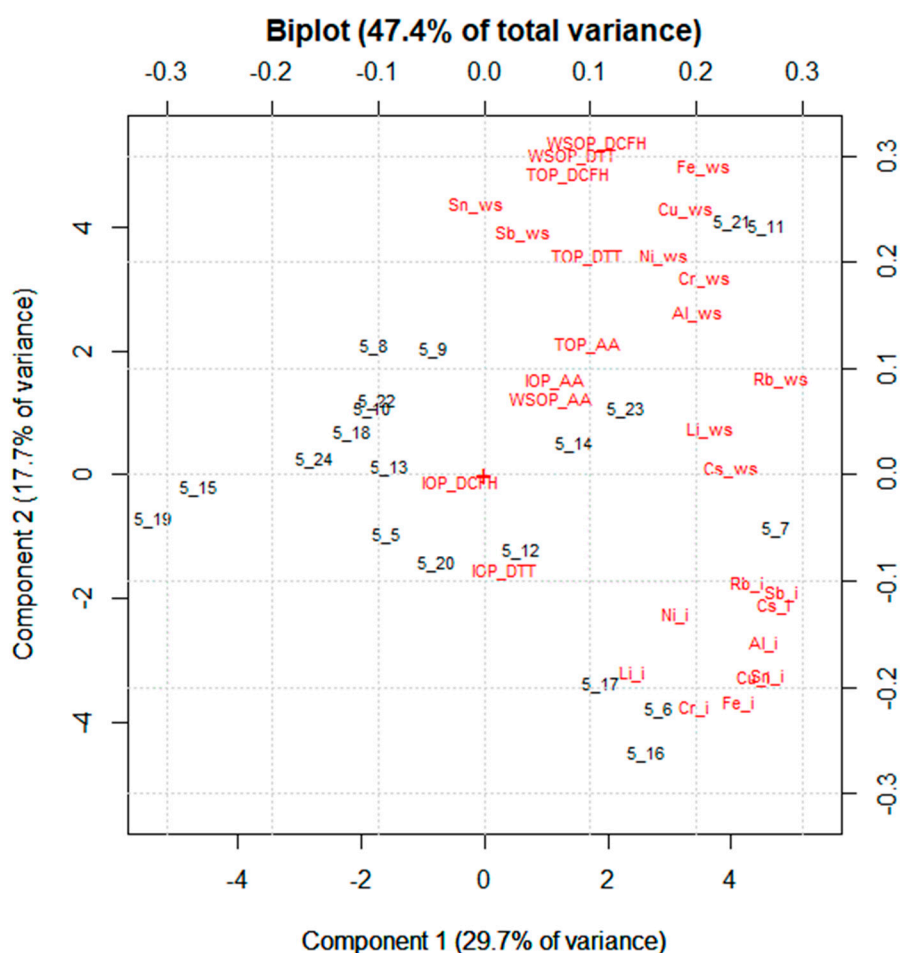


Figure S1. Biplot of PC1/PC2 from the PCA performed on the WSOP, TOP and IOP values for OP^{AA}, OP^{DTT} and OP^{DCFH}, and element concentrations in the water-soluble (_ws) and insoluble (_i) fraction of the 20 PM₁₀ samples.

Table S1. Scores and loadings of the five significant components obtained by performing the PCA on the matrix of the data (580 data points) composed of 20 PM₁₀ samples and 29 variables.

Sampling days	Scores				
	PC1	PC2	PC3	PC4	PC5
05/05/2021	-1.58623	-0.97751	0.366896	-0.58442	0.525427
06/05/2021	2.825923	-3.78792	3.093845	0.545744	-0.39122
07/05/2021	4.723902	-0.86232	-1.14036	-2.10932	-1.13162
08/05/2021	-1.8033	2.084004	-1.30369	1.441808	1.868484
09/05/2021	-0.83201	2.034397	-1.10832	-0.01011	0.298175
10/05/2021	-1.80823	1.050559	-0.8631	0.088544	-1.31561
11/05/2021	4.579853	4.018884	2.279596	2.541445	0.896487
12/05/2021	0.582918	-1.23078	-0.27615	-2.92858	-0.90267
13/05/2021	-1.53575	0.115022	-0.13071	-1.83719	-0.55313
14/05/2021	1.459193	0.496354	-3.52565	-0.42523	2.837427
15/05/2021	-4.62859	-0.20388	0.716007	-1.35113	-0.341
16/05/2021	2.620193	-4.48785	-4.05242	1.277222	1.632599
17/05/2021	1.889916	-3.38443	3.736475	0.667041	0.574365
18/05/2021	-2.15952	0.67568	1.173823	-1.38265	0.085947
19/05/2021	-5.36124	-0.71588	0.568159	1.140972	0.694384
20/05/2021	-0.78153	-1.41344	0.723884	1.187126	0.323789
21/05/2021	4.018949	4.075919	1.394198	-2.57333	1.033031
22/05/2021	-1.73454	1.199607	1.05762	2.003	0.199001
23/05/2021	2.296258	1.06587	-2.21067	2.274585	-4.77111
24/05/2021	-2.76617	0.247707	-0.49945	0.03448	-1.56275

Variables	Loadings				
	PC1	PC2	PC3	PC4	PC5
Al_ws	0.202118	0.152137	0.112682	0.119205	0.189423
Cr_ws	0.209275	0.185106	-0.09756	0.025169	-0.26846
Cs_ws	0.233754	0.005509	0.198207	-0.25518	0.158213
Cu_ws	0.191098	0.250126	-0.15696	-0.22041	0.000476
Fe_ws	0.207767	0.289439	-0.01825	0.151439	-0.04107
Li_ws	0.213234	0.043432	0.268443	-0.16677	0.013301
Ni_ws	0.170286	0.204958	-0.23076	-0.22054	0.124316
Rb_ws	0.281455	0.09039	0.171594	-0.02445	0.019824
Sb_ws	0.037206	0.226891	-0.03177	0.263081	-0.11452
Sn_ws	-0.007	0.254486	-0.13573	0.191646	0.278418
Al_i	0.263753	-0.15869	0.168546	0.152362	-0.15281
Cr_i	0.198209	-0.21885	-0.25667	0.080872	0.074766
Cs_i	0.273661	-0.12257	0.211103	0.03386	-0.12215
Cu_i	0.25519	-0.19079	-0.19718	-0.09994	0.133902
Fe_i	0.240169	-0.21497	-0.20856	0.043342	0.052501
Li_i	0.13994	-0.18706	0.30071	0.113352	-0.05304
Ni_i	0.180699	-0.1324	-0.28278	-0.06543	0.272648
Rb_i	0.248643	-0.10284	0.15529	0.088082	-0.21192
Sb_i	0.281863	-0.1117	-0.10927	0.076375	-0.05547
Sn_i	0.268744	-0.18949	-0.11911	5.76E-05	0.156959
WSOP_DCFH	0.106592	0.31247	0.003721	0.282605	0.122929
WSOP_AA	0.080588	0.282404	0.244534	-0.01092	0.080655
WSOP_DTT	-0.02158	-0.00766	0.29737	-0.332	-0.04064

TOP_DCFH	0.064564	0.070874	-0.00942	-0.47377	-0.23155
TOP_AA	0.098635	0.122204	-0.15466	-0.02628	-0.48675
TOP_DTT	0.066954	0.088444	-0.16027	0.25711	-0.38284
IOP_DCFH	0.083487	0.300087	-0.07867	-0.19464	0.064812
IOP_AA	0.09791	0.205504	0.161367	0.05422	0.221876
IOP_DTT	0.019403	-0.0906	0.259459	0.264108	0.174796

Table S2. Results of this study compared with other findings available in the literature.

References	Performed OP assays	PM aerodynamic diameter	Main findings
This study	OP ^{DCFH} OP ^{AA} OP ^{DTT}	PM ₁₀	Water-soluble PM is mainly responsible for the generation of the TOP. Insoluble PM from mineral dust contribute to the IOP ^{DCFH} and IOP ^{DTT}
Frezzini et al., 2022 [42]	OP ^{DCFH} OP ^{AA} OP ^{DTT}	PM ₁₀	The redox activity of the insoluble fraction of PM provided a significant contribution to the OP ^{AA}
Gao et al., 2020 [15]	OP ^{DTT}	PM _{2.5}	Water-insoluble PM contributed $\approx 20\%$ to the OP of particles
Wang et al., 2013 [43]	Macrophage ROS assay (DCFH)	Coarse PM _{2.5} Ultrafine	Insoluble fraction played a key role in potential toxicity of PM
Verma et al., 2012 [45]	OP ^{DTT}	PM _{2.5}	Hydrophobic fraction of insoluble organic aerosols contributed to the oxidative properties of ambient PM
Daher et al., 2011 [40]	OP ^{DTT} Dihydroxybenzoate (DHBA)	PM _{2.5}	Insoluble PM species emerged as potentially redox active