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Distribution and stable carbon isotopic composition of dicarboxylic acids, ketocarboxylic acids and α-dicarbonyls in fresh and aged biomass burning aerosols

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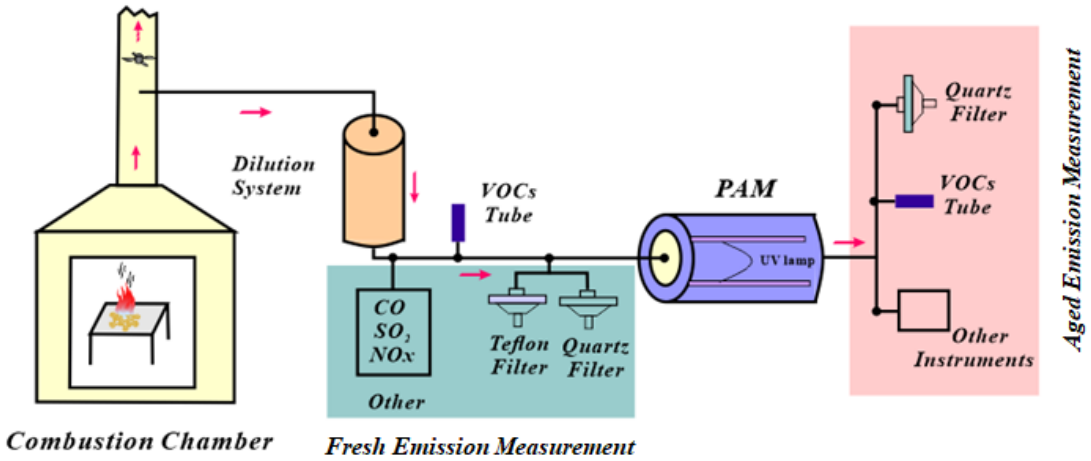

Figure S1 Schematic diagram of biomass burning simulation experiments (originally published as supplement in Li et al. (2021).

Table S1 Emission factors (EFs) of fresh and aged dicarboxylic acids and related compounds from biomass burning (mg kg^{-1}) and the ratio of aged/fresh

Compounds	Fresh	2-day aged	7-day aged	2-day aged/fresh	7-day aged/fresh
I. Dicarboxylic acids					
Oxalic, C_2	18 ± 6.7	930 ± 214	1180 ± 337	50.8	64.5
Malonic, C_3	4.3 ± 3.7	69 ±18	133 ± 40	16.2	31.1
Succinic, C_4	44 ± 25	252 ± 65	352 ± 109	5.7	8.0
Glutaric, C_5	16 ± 7.7	35 ± 12	32 ± 10	2.2	2.1
Adipic, C_6	6.4 ± 1.4	31 ± 8.7	31 ± 10	4.9	4.8
Pimelic, C_7	6.0 ± 3.9	15 ± 2.6	7.6 ± 1.6	2.5	1.3
Azelaic, C_9	18 ± 7.3	51 ± 14	39 ± 16	2.8	2.2
Sebacic, C_{10}	5.2 ± 2.1	5.9 ± 2.8	/	1.1	/
Undecanedioic, C_{11}	7.7 ± 1.4	13 ± 1.9	21 ± 7.4	1.7	2.8
Methylmalonic, iC_4	8.1 ± 2.3	9.7 ± 8.4	22 ± 6.8	1.2	2.8
Mehtylsuccinic, iC_5	5.3 ± 1.5	82 ± 48	23 ± 9.2	15.4	4.3
Methylglutaric, iC_6	4.4 ± 2.2	10 ±3.0	16 ± 9.4	2.3	3.7
Maleic, M	4.3 ± 1.0	34 ± 9.0	24 ± 6.0	7.9	5.6
Fumaric, F	6.0 ± 0.7	46 ± 14	24 ± 19	7.8	4.0
Methylmaleic, mM	7.5 ± 4.5	12 ± 3.6	9.4 ± 2.8	1.6	1.2
Phthalic, Ph	8.5 ± 5.6	33 ± 8.0	20 ± 6.2	3.9	2.4
Isophthalic, iPh	5.6 ± 2.4	13.5 ± 3.4	15 ± 5.2	2.4	2.7
Ketopimelic, kC_7	6.1 ± 2.5	6.7 ± 1.7	7.1 ± 1.9	1.1	1.2
Subtotal	181 ± 82	1650 ± 438	1957 ± 598	9.1	10.8
II. Ketocarboxylic acids					
Pyruvic, Pyr	11 ± 6.6	157 ± 27	124 ± 51	14.1	11.1
Glyoxylic, ωC_2	18 ± 6.6	245 ± 33	225 ± 63	13.5	12.4
Subtotal	29 ± 13	403 ± 60	349 ± 114	13.8	11.9
III. α-Dicarbonyls					
Glyoxal, Gly	51 ± 18	297 ± 82	174 ± 53	5.8	3.4
Methylglyoxal, mGly	27 ± 20	125 ± 33	83 ± 24	4.6	3.1
Subtotal	78 ± 38	423 ± 114	257 ± 76	5.4	3.3
Benzoic, Ha	2.5 ± 0.3	20 ± 22	4.6 ± 1.2	7.9	1.9
Total detected	291 ± 132	2495 ± 634	2568 ± 790	8.6	8.8

Table S2 Stable carbon isotope ratios ($\delta^{13}C$, ‰) of C_3, C_4 and ωC_2 in the 2- and 7-day aged $PM_{2.5}$ aerosols from the burning of rice, maize, and wheat straws

Compounds	Sampling time	Straw type	Range	Mean (SD)
C_3	2-day aged	Maize straw	-9.7 to -7.8	-8.4 (1.1)
		Rice straw	-22.5 to -18.3	-21.0 (2.3)
		Wheat straw	-27.7 to -26.6	-27.0 (0.5)
	7-day aged	Maize straw	-1.4 to 6.4	2.8 (3.3)
		Rice straw	-18.8 to -11.4	-15.3 (3.7)
		Wheat straw	-22.0 to -20.5	-21.2 (0.8)
	2-day aged	Biomass burning	-20.0 to -17.6	-18.8 (1.3)
	7-day aged	Biomass burning	-14.1 to -8.5	-11.2 (2.6)
C_4	2-day aged	Maize straw	-12.4 to -10.5	-11.3 (1.0)
		Rice straw	-24.4 to -22.6	-23.8 (1.0)
		Wheat straw	-27.1 to -26.0	-26.4 (0.6)
	7-day aged	Maize straw	-9.1 to -7.0	-7.7 (1.0)
		Rice straw	-24.0 to -21.5	-22.6 (1.3)
		Wheat straw	-24.7 to -21.9	-23.0 (1.4)
	2-day aged	Biomass burning	-21.3 to -9.7	-20.5 (0.9)
	7-day aged	Biomass burning	-19.3 to -16.8	-17.8 (1.2)
ωC_2	2-day aged	Maize straw	-5.1 to -4.9	-5.0 (0.1)
		Rice straw	-19.2 to -16.8	-17.7 (1.3)
		Wheat straw	-19.5 to -17.6	-18.3 (1.1)
	7-day aged	Maize straw	3.5 to 10.5	6.0 (3.2)
		Rice straw	-9.0 to -1.7	-6.5 (4.1)
		Wheat straw	-17.1 to -16.1	-18.3 (1.1)
	2-day aged	Biomass burning	-14.6 to -13.1	-13.7 (0.8)
	7-day aged	Biomass burning	-7.5 to -2.4	-6.3 (2.8)

39 Table S3 Correlation coefficients (R) between increases in dicarboxylic acids and decreases in VOCs from rice, maize and wheat straw 2-day aged burning samples

	C_2	C_3	C_4	Pyr	ωC_2	Gly	Ethylene	Propylene	trans-2-Butene	cis-2-Butene	1-Pentene	Isoprene	trans-2-Pentene	cis-2-Pentene	1-Hexene	n-Butane	iso-Pentane	Cyclohexane	Methylcyclohexane	Benzene	Toluene
C_2	1																				
C_3	0.48	1																			
C_4	0.46	0.95*	1																		
Pyr	0.80*	0.83*	0.86**	1																	
ωC_2	0.85**	0.73*	0.76*	0.97**	1																
Gly	0.74*	0.88*	0.87*	0.95**	0.94**	1															
Ethylene	0.52	0.39	0.34	0.64	0.58	0.48	1														
Propylene	0.69*	0.60	0.47	0.59	0.69*	0.75*	0.12	1													
trans-2-Butene	0.52	0.76*	0.63	0.66	0.68*	0.80**	0.24	0.92**	1												
cis-2-Butene	0.69	0.73*	0.61	0.60	0.63	0.75*	0.20	0.88**	0.98**	1											
1-Pentene	0.61	0.69*	0.57	0.57	0.58	0.72*	0.15	0.86**	0.98**	0.98**	1										
Isoprene	0.25	0.22	0.11	-0.01	0.01	0.08	-0.40	0.47	0.43	0.43	0.44	1									
trans-2-Pentene	0.76*	0.70*	0.57	0.64	0.67*	0.76*	0.18	0.91**	0.94**	0.89**	0.91**	0.62	1								
cis-2-Pentene	0.56	0.58	0.42	0.43	0.48	0.59	-0.09	0.89**	0.81**	0.75*	0.77*	0.78*	0.92**	1							
1-Hexene	0.55	0.68*	0.48	0.53	0.56	0.72*	0.15	0.94**	0.94**	0.88**	0.89**	0.45	0.91**	0.88**	1						
n-Butane	0.50	0.70*	0.50	0.60	0.57	0.71*	0.35	0.75*	0.72*	0.61	0.62	0.27	0.76*	0.75*	0.86**	1					
iso-Pentane	0.56	0.69*	0.66	0.76*	0.71*	0.75*	0.34	0.63	0.62	0.56	0.59	0.01	0.61	0.48	0.62	0.73*	1				

Cyclohexane	0.48	0.54	0.44	0.55	0.61	0.62	0.15	0.71*	0.52	0.39	0.37	0.26	0.61	0.71*	0.69*	0.83**	0.54	1		
Methylcyclohexane	0.55	0.39	0.31	0.63	0.66	0.61	0.58	0.45	0.30	0.16	0.15	-0.22	0.36	0.31	0.44	0.74*	0.65	0.78*	1	
Benzene	0.52	0.28	0.24	0.37	0.43	0.37	-0.13	0.60	0.35	0.27	0.29	0.60	0.59	0.74*	0.46	0.55	0.54	0.69*	0.49	1
Toluene	0.67*	0.62	0.44	0.59	0.63	0.75*	0.25	0.88**	0.83**	0.72*	0.76*	0.37	0.89**	0.85**	0.93**	0.92**	0.62	0.82**	0.64	0.57	1

Note: See Table 1 for abbreviations

** Correlation is significant at the 0.01 level (2 tailed).

* Correlation is significant at the 0.05 level (2 tailed).

40

Reference

Li, J. J., Li, J., Wang, G. H., Ho, K. F., Dai, W. T., Zhang, T., Wang, Q., Wu, C., Li, L., Li, L., and Zhang, Q.: Effects of atmospheric aging processes on in vitro induced oxidative stress and chemical composition of biomass burning aerosols, J. Hazard. Mater., 401, 123750, https://doi.org/10.1016/j.jhazmat.2020.123750, 2021.