

1 **Supplementary Information**

2
3 **Distribution and stable carbon isotopic compositions of dicarboxylic**
4 **acids, ketocarboxylic acids and α -dicarbonyls in fresh and aged**
5 **biomass burning aerosols**

6 Minxia Shen^{1,2}, Kin Fai Ho^{3,4}, Wenting Dai¹, Suixin Liu¹, Ting Zhang¹, Qiyuan Wang¹,
7 Jingjing Meng⁵, Judith C. Chow^{1,6}, John G. Watson^{1,6}, Junji Cao^{1*}, Jianjun Li^{1,7*}

8
9 ¹State Key Laboratory of Loess and Quaternary Geology, Key Lab of Aerosol
10 Chemistry and Physics, Institute of Earth Environment, Chinese Academy of
11 Sciences, Xi'an 710061, China;

12 ²University of Chinese Academy of Sciences, Beijing, China;

13 ³The Jockey Club School of Public Health and Primary Care, The Chinese University
14 of Hong Kong, Hong Kong, China;

15 ⁴Shenzhen Municipal Key Laboratory for Health Risk Analysis, Shenzhen Research
16 Institute, The Chinese University of Hong Kong, Shenzhen, China;

17 ⁵ School of Geography and the Environment, Liaocheng University, Liaocheng
18 252000, China;

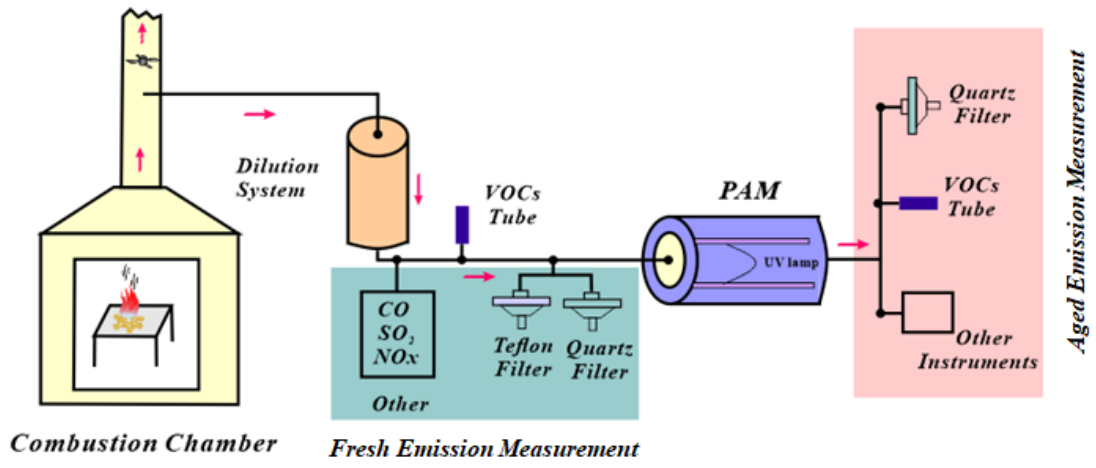
19 ⁶Division of Atmospheric Sciences, Desert of Research Institute, Reno, Nevada, USA

20 ⁷CAS Center for Excellence in Quaternary Science and Global Change, Xi'an 710061,
21 China.

22
23
24
25 **Corresponding author: Jianjun Li, e-mail address:*lijj@ieecas.cn

26 *Junji Cao, e-mail address:*cao@loess.llqg.ac.cn;

27



28
29
30
31
32

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

33 Table S1 Emission factors (EFs) of fresh and aged dicarboxylic acids and related compounds from
 34 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
Methylsuccinic, 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

35

36

37 Table S2 Stable carbon isotope ratios ($\delta^{13}\text{C}$, ‰) of C_3 , C_4 and ωC_2 in the 2- and 7-day aged $\text{PM}_{2.5}$
 38 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)	
	C_4	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)
		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)	
ωC_2		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)	
	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	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
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**	0.57

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).

41 **Reference**

42 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
43 Zhang, Q.: Effects of atmospheric aging processes on in vitro induced oxidative stress and
44 chemical composition of biomass burning aerosols, *J. Hazard. Mater.*, 401, 123750,
45 <https://doi.org/10.1016/j.jhazmat.2020.123750>, 2021.

46