Supporting information

Protein amino acids in fine and coarse atmospheric aerosol: concentrations, compositions, sources and possible bacterial

degradation state

Ren-guo Zhu¹, Hua-Yun Xiao^{2, 1*}, Li Luo¹, Hongwei Xiao¹, Zequn Wen³, Yuwen Zhu^{1,} ⁴, Xiaozheng Fang¹, Yuanyuan Pan¹, Zhenping Chen¹

1 Jiangxi Province Key Laboratory of the Causes and Control of Atmospheric Pollution, East China University of Technology, Nanchang 330013, China.

2 School of Environmental Science and Engineering, Shanghai Jiao Tong University, Shanghai 200240, China

3 Department of Earth Sciences, Faculty of Land Resource Engineering, Kunming University of Science and Technology, Kunming 650021, China

4 School of Earth Sciences, East China University of Technology, Nanchang 330013, China;

Corresponding author: Hua-Yun Xiao (xiaohuayun@ecut.edu.cn)



Figure S1. Concentrations of THAA for fine (F) and coarse (C) particles in airport, urban, forest, town and suburban sites (a) and Concentrations of THAA for fine and coarse particles on rainy and dry days(b). Red box indicates fine particles and green box indicates coarse particles. The box encloses 50% of the data, the whisker is standard deviation of the data, the horizontal bar is the median, solid circles are outliers. In a, different uppercase letters denote means found to be statistically different between sites and different lower case letters denote means found to be statistically different between fine and coarse particles (two-way ANOVA, p < 0.05). In b, different uppercase letters denote means found to be statistically different lower case letters denote means found to be statistically different lower case letters denote means found to be statistically different between fine and coarse particles (two-way ANOVA, p < 0.05). In b, different and dry days (two-way ANOVA, p < 0.05). In order to make graph more visual clarity, a zero-line were added.



Figure S2. Average contributions of HAA species with high abundance in natural sources (hydrophobic (Ala, Val, Leu, and Ile), neutral (Pro) and hydrophilic (Glu, Lys, and Asp)) to total

HAAs during 14 consecutive sampling days.



Figure S3. Comparison of DI values obtained by principal component analysis (this study) with those calculated by using the coefficients reported by Dauwe et al., 1999 and Yamashia and Tanoue, 2003. Red box indicates fine particles and blue box indicates coarse particles. The box encloses 50% of the data, the whisker is standard deviation of the data, the horizontal bar is the median, solid circles are outliers. Identical uppercase letters denote DI means found to be not statistically different between different calculating methods and different lower case letters denote means found to be statistically different between fine and coarse particles (two-way ANOVA, p < 0.05).



Figure S4. DI values for fine and coarse particles in urban, town, suburban airport and forest sites. The box encloses 50% of the data, the whisker is standard deviation of the data, the horizontal bar is the median, solid circles are outliers. Different uppercase letters denote means found to be statistically different between fine and coarse particles (two-way ANOVA, Tukey-HSD test, p < 0.05). Identical lower case letters denote means found to be not statistically different between sites.



Figure S5. The 2-day (48 h) back trajectories at 500m height illustrating the typical air mass flows to the sampling site (28.85°N, 115.91°E) during the sampling periods. The map comes from the MeteoInfoMap (version 1.4.9R2) software (Chinese Academy of Meteorological Sciences, China).

Compo nent	Initial Eigenvalues			Extraction Sums of Squared Loadings		
	Total	% of Variance	Cumulative %	Total	% of Variance	Cumulative %
1	5.360	38.286	38.286	5.360	38.286	38.286
2	2.926	20.899	59.185	2.926	20.899	59.185
3	1.335	9.534	68.719	1.335	9.534	68.719
4	1.074	7.670	76.388	1.074	7.670	76.388
5	.858	6.127	82.515			
6	.732	5.232	87.747			
7	.593	4.233	91.979			
8	.481	3.438	95.417			
9	.304	2.169	97.586			
10	.170	1.211	98.798			
11	.111	.791	99.588			
12	.031	.221	99.810			
13	.027	.190	100.000			
14	-4.620E-16	-3.300E-15	100.000			

Table S1. Result of principal component analysis. For each PC with an eigenvalue >1, eigenvalues, percent of variation explained (%), cumulative variation explained (Cumulative%) are listed.

Extraction Method: Principal Component Analysis.

Table S2. Result of principal component analysis (PCA). PC loadings (eigenvectors) for each AA are listed.

	Component						
	1	2	3	4			
Ala	.143	138	159	067			
Gly	.087	.105	.175	423			
Val	.132	233	038	.072			
Leu	.133	228	.031	.082			
lle	.138	212	.011	.092			
Pro	180	.001	056	.134			
Ser	.096	.229	185	.133			
Thr	.071	.112	204	295			
Phe	.120	.124	140	102			
Asp	.094	.164	152	.070			
Glu	.137	.180	.074	.016			
Lys	.119	.108	.341	.220			
His	.023	.053	.636	.160			
Tyr	.026	.082	205	.718			

Component Score Coefficient Matrix

Extraction Method: Principal Component Analysis.

Component Scores.