Supporting information for:

Aggregation-Induced Emission Micelle-Based Sensing Array for Discrimination of Long-Chain Fatty Acids

Bingqian Yan,[†] Yunxiu Jia,[†] Xin Zhang,[‡] Lijuan Zhang,*[,†] Weijiang Guan*[,†] and Chao Lu*[,†,§]

[†]*State Key Laboratory of Chemical Resource Engineering, Beijing University of Chemical Technology, Beijing 100029, China.*

[‡]*Department of Chemistry, Capital Normal University, Beijing, 100048, China.*

[§]*Pingyuan Laboratory, College of Chemistry, Zhengzhou University, Zhengzhou, 450001, China.*

Experimental section

Chemicals and materials. Lauric acid, palmitic acid, and stearic acid were purchased from J&K Scientific (Beijing, China). Tetrahydrofuran (THF) was purchased from Beijing chemical (Beijing, China). C_8-TPE-C_4TAB, C_4-TPE-C_8TAB, and TPE-C_{12}TAB were synthesized based on our previous work.[20] Deionized water used throughout the experiments was purified by a Milli-Q Advantage A10 water purification system (Merck Millipore, Germany). All chemicals were of analytical reagent grade and used as received without any further purification.

Preparation of different fatty acid stock solutions A auric acid stock solution (10 mM), a palmitic acid stock solution (10 mM), and a stearic acid stock (10 mM) solution were prepared by weighing 10.0 mg of lauric acid, 12.9 mg of palmitic acid, and 14.2 mg of stearic acid and dissolving them in 5 mL of tetrahydrofuran, respectively.

Fluorescence response of different probes to fatty acids. The three fatty acid stock solutions were diluted with tetrahydrofuran to a gradient concentration of 1 to 7 mM, respectively. The above gradient concentrations of fatty acid solutions were added to the solutions of C_8-TPE-C_4TAB (90 μM), C_4-TPE-C_8TAB (90 μM) and TPE-C_{12}TAB (90 μM) at a volume ratio of 1:100, respectively. Finally, the mixed solutions were treated by ultrasound for 5 min, followed by fluorescence measurements.

Array-based sensing of fatty acids. To identify the fatty acids (70 μM), the different kinds of fatty acid stock solutions were diluted to 7 mM and added to 90 μM of C_8-TPE-C_4TAB, C_4-TPE-C_8TAB, and TPE-C_{12}TAB solutions at a volume ratio of 1:100, respectively, and their fluorescence spectra were measured. The fluorescence change, $(I-I_0)/I_0$, was calculated and utilized for the linear discriminant analysis (LDA). I_0 and I indicate the emission intensity of the AIE micelles in the absence and presence of fatty acids. The analysis was repeated 10 times for the three fatty acids. Three tests were

performed against three AIE micelle arrays of three fatty acids to provide a 3 × 3 × 10 matrix of training data. The emission intensity of AIE micelle arrays at the maximum wavelength was selected during all LDA processing. For the distinction of 30 μM fatty acids, each AIE micelle solution was mixed with a 3 mM fatty acid solution. For the distinction of the mixed fatty acids, 3 mM fatty acid solutions were mixed in a certain ratio and the mixed solutions were added into C_8-TPE-C_4TAB (90 μM), C_4-TPE-C_8TAB (90 μM), and TPE-C_{12}TAB (90 μM) solutions at a volume ratio of 1:100, and the fluorescence spectra were recorded after ultrasonication and analyzed by LDA. The fluorescence response pattern was generated using the maximum emission relative integrated fluorescence intensity change, i.e. $(I-I_0)/I_0$.

Characterizations. Fluorescence spectra were got on a F-7000 spectrophotometer (Hitachi, Japan). The slit width was 5 nm and the scanning rate was kept at 2400 nm/min. UV-Vis absorption spectra were acquired on a UV-3600 spectrophotometer (Shimadzu, Japan) with detection wavelength ranging from 220 to 800 nm.

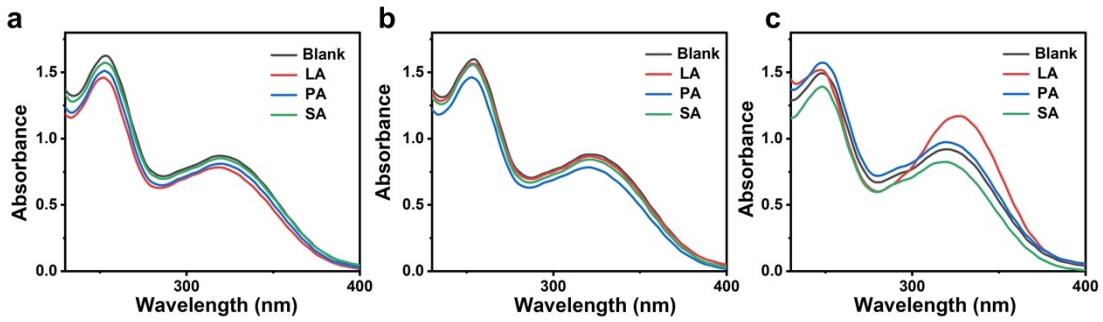

Fig. S1 UV-Vis absorption spectra of (a) C_8-TPE-C_4TAB micelles, (b) C_4-TPE-C_8TAB micelles, and (c) TPE-C_{12}TAB micelles in the presence of 70 μM LA, PA, and SA.

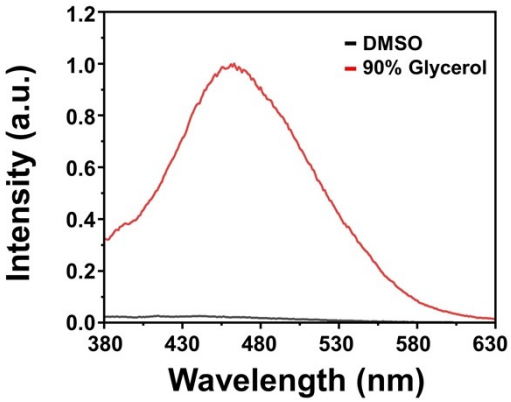

Fig. S2 Fluorescence spectra of TPE in DMSO solution and 90% glycerol solution.

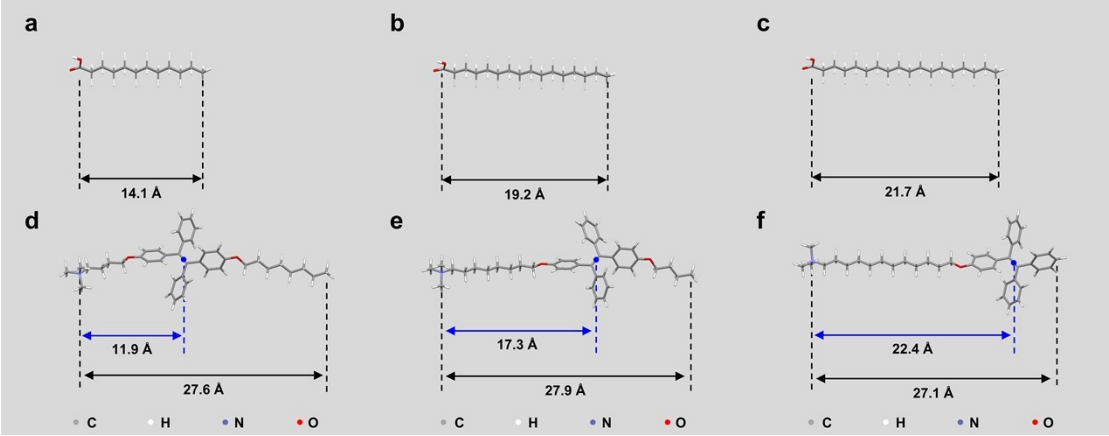

Fig. S3 The energy-minimized molecular structures of (a) LA, (b) PA, (c) SA, (d) C_8-TPE-C_4TAB, (e) C_4-TPE-C_8TAB, and (f) TPE-C_{12}TAB. Note that the structures shown in d-f are those we have published in *Angew. Chem. Int. Ed.*, 2021, **60**, 13029.

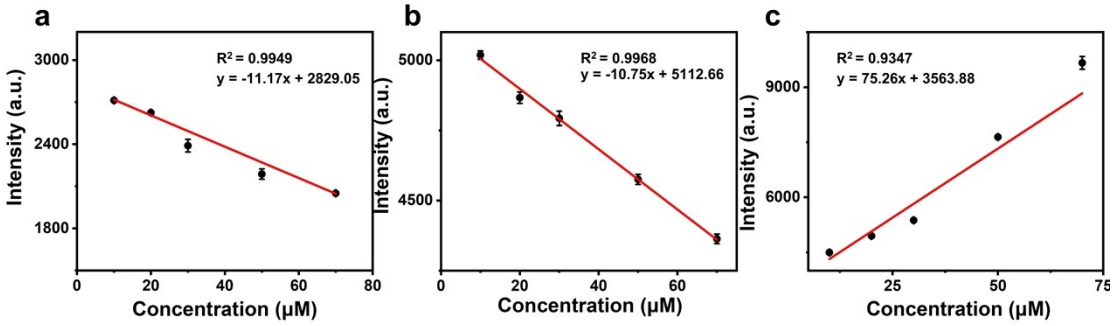

Fig. S4 The fluorescence changes of the three AIE micelles were plotted linearly against the concentration of LA in the range of 0–70 μM.

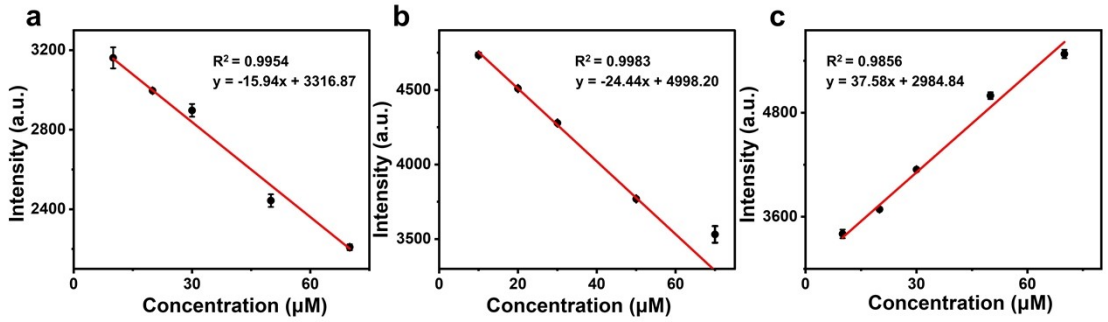

Fig. S5 The fluorescence changes of the three AIE micelles were plotted linearly against the concentration of PA in the range of 0–70 μM.

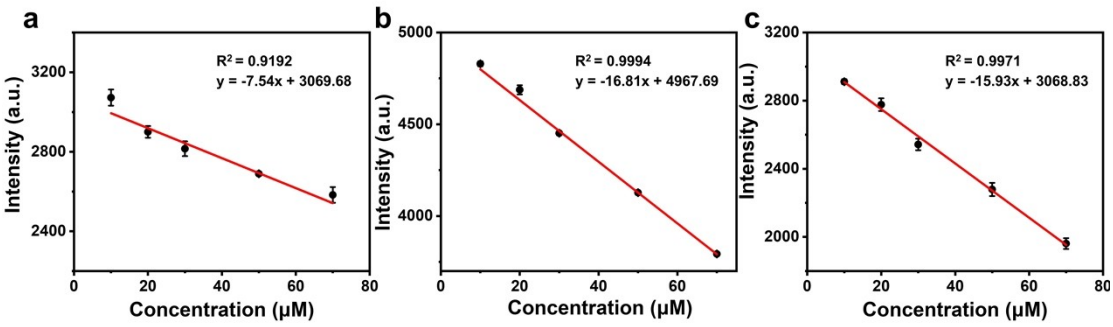

Fig. S6 The fluorescence changes of the three AIE micelles were plotted linearly against the concentration of SA in the range of 0–70 μM.

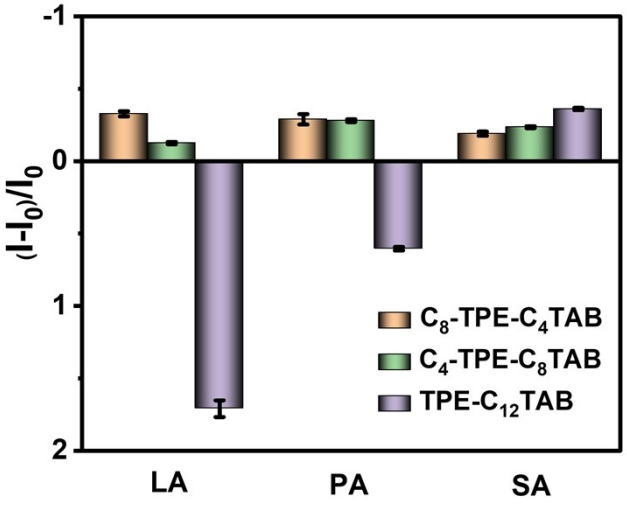

Fig. S7 Relative fluorescence [$(I-I_0)/I_0$] values of the AIE micelle-based array upon the addition of 70 μM LA, 70 μM PA, and 70 μM SA, respectively. Values were obtained as the average of 10 parallel measurements.

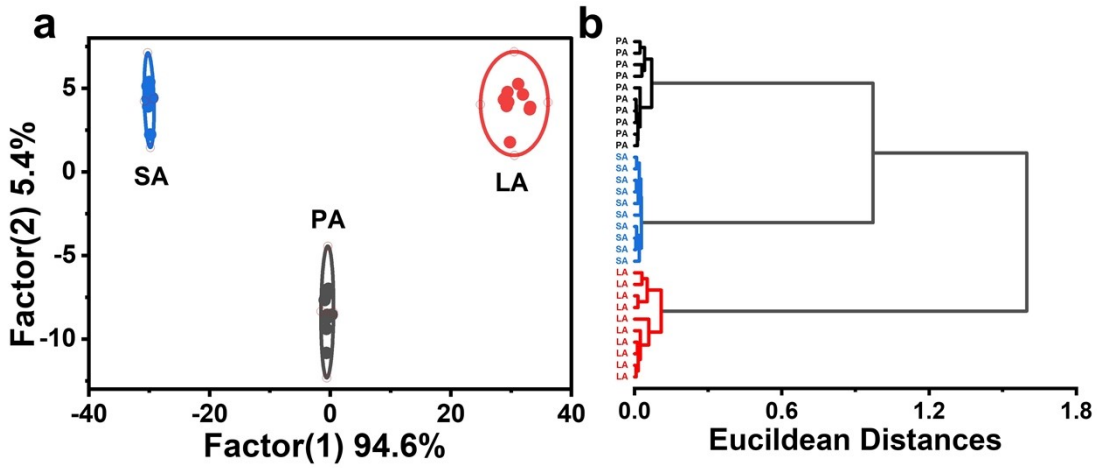

Fig. S8 (a) Canonical score plots for the first two factors of relative fluorescence [$(I-I_0)/I_0$] patterns from three fatty acids analyzed by LDA. (b) The corresponding HCA analysis with 10 parallel measurements.

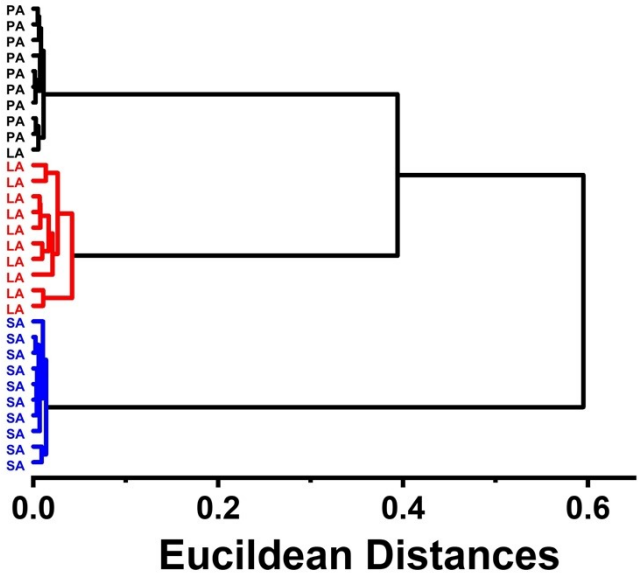

Fig. S9 The corresponding HCA analysis with 10 parallel measurements for **Fig. 2**.

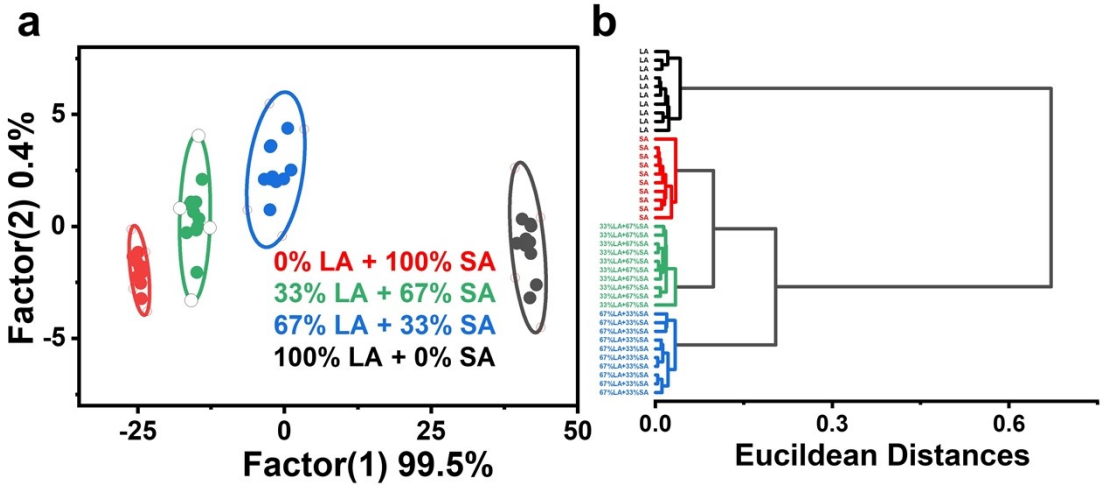

Fig. S10 (a) Canonical score plots for the first two factors of relative fluorescence [$(I-I_0)/I_0$] patterns from the mixtures of LA and SA analyzed by LDA. (b) The corresponding HCA analysis with 10 parallel measurements.

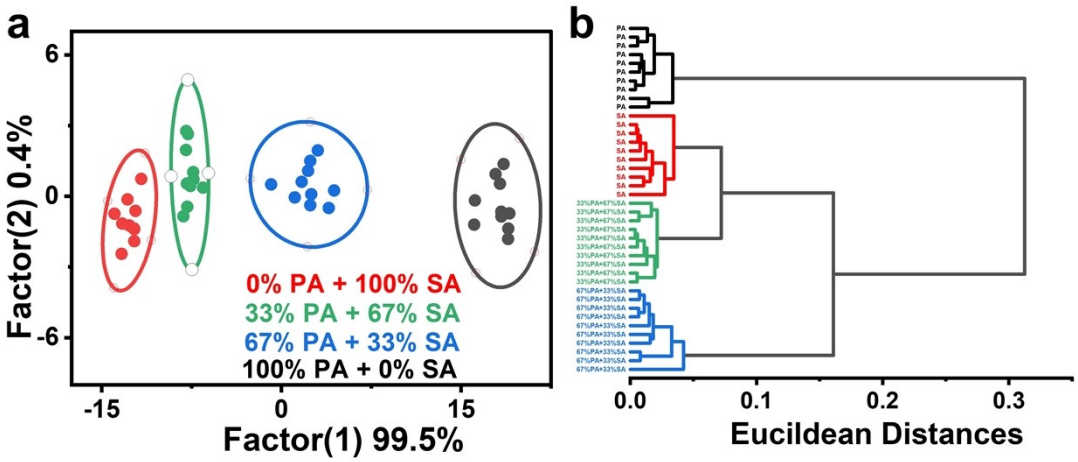

Fig. S11 (a) Canonical score plots for the first two factors of relative fluorescence [$(I-I_0)/I_0$] patterns from the mixtures of PA and SA analyzed by LDA. (b) The corresponding HCA analysis with 10 parallel measurements.

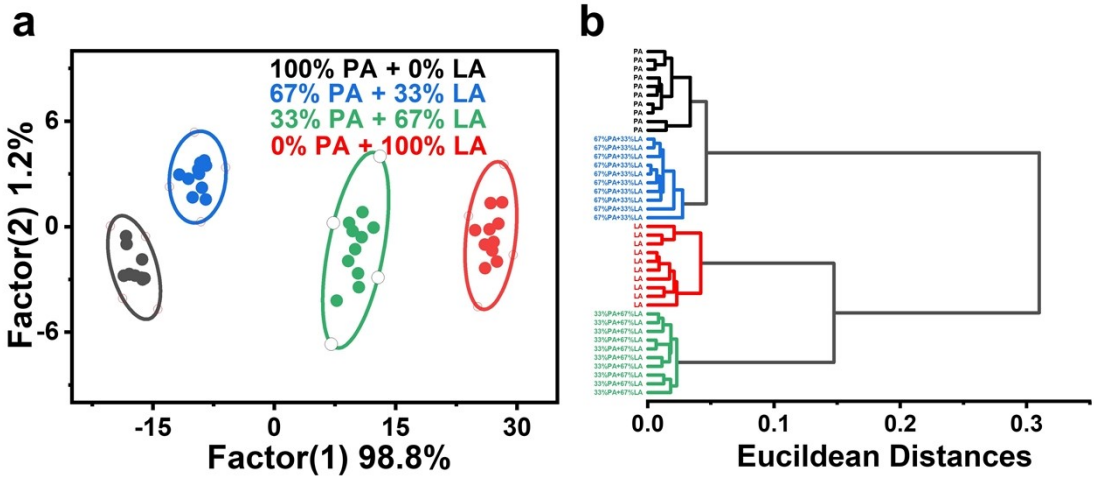

Fig. S12 (a) Canonical score plots for the first two factors of relative fluorescence [$(I-I_0)/I_0$] patterns from the mixtures of PA and LA analyzed by LDA. (b) The corresponding HCA analysis with 10 parallel measurements.

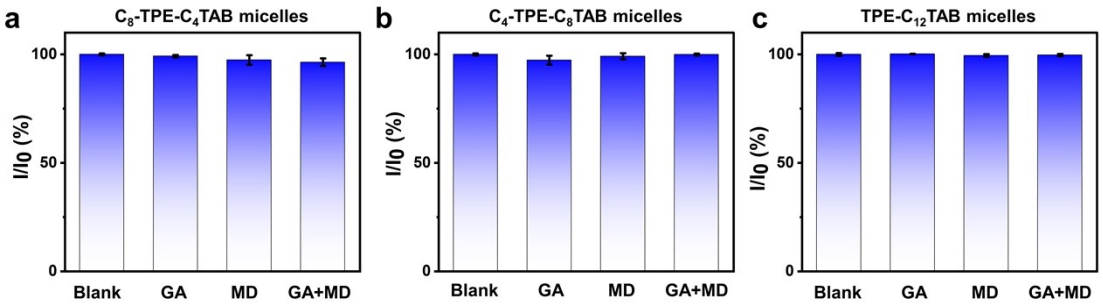

Fig. S13 Relative fluorescence I/I_0 values of (a) C_8-TPE-C_4TAB micelles, (b) C_4-TPE-C_8TAB micelles, and (c) TPE-C_{12}TAB micelles in the presence of 5 mg/mL GA, 5 mg/mL MD, and their 1:1 mixture.

Table S1. Method for mixing the three fatty acids (Total concentration = 30 μM).

LA%	PA%	SA%	Total%
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
20	20	60	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
40	40	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
60	20	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
20	60	20	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100
33	33	33	100

Table S2. Results for PLS regression.

	R^2	RMSE[a]	R^2 CV	RMSECV[b]
LA	0.898	0.0474	0.854	0.0568
PA	0.984	0.0186	0.976	0.0228
SA	0.939	0.0384	0.915	0.0453

[a]Root Mean Square Error (RMSE), [b]Root Mean Square Error Cross-validation (RMSECV).