SUPPORTING INFORMATION

A Non-Invasive Strategy Based on Real-time in Vivo Cataluminescence Monitoring for Clinical Breath Analysis

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Content

1. The Relationship between Pressure and Flow Rate

As shown in Figure S1, a well linear relationship between the pressure and flow rate with a correlation coefficient of 0.9988 was observed.

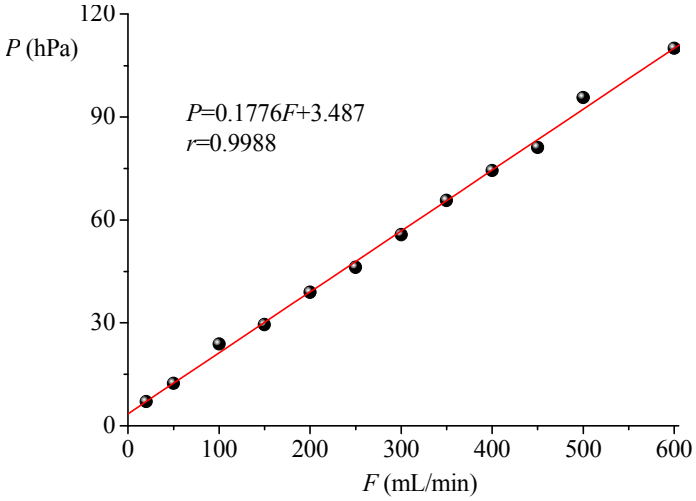

Figure S1. The relationship between pressure and flow rate.

2. Flow Chart of the Strategy

The flow chart of the strategy proposed by the present work are shown in Figure S2.

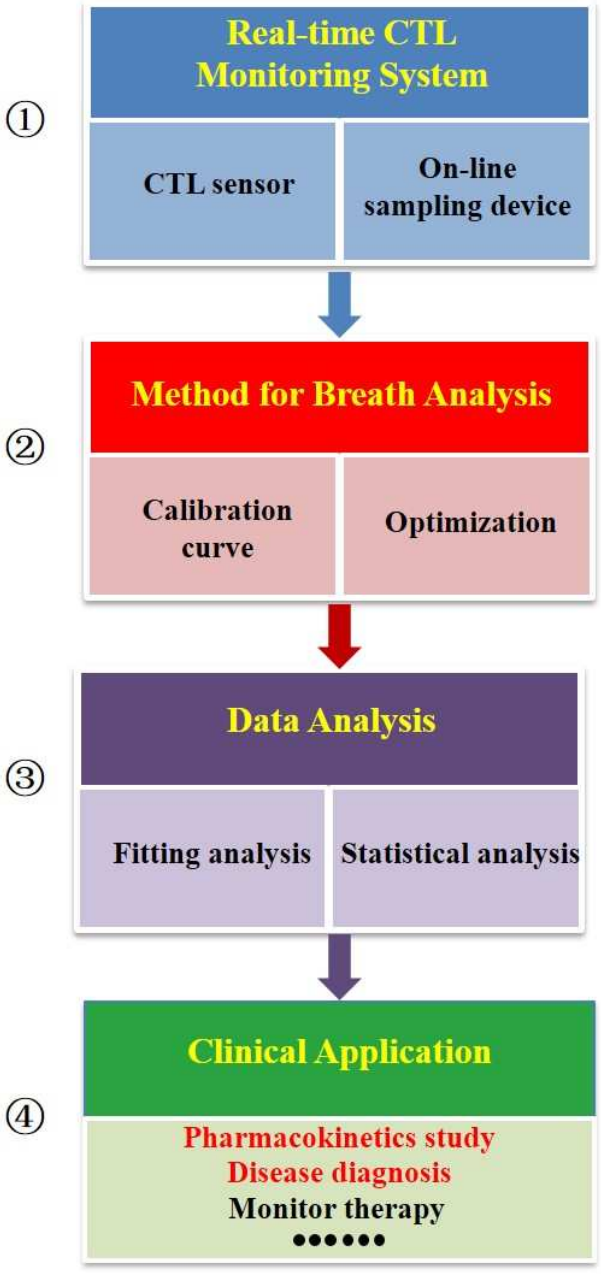

Figure S2. The flow chart of the strategy

3. The Stability and Moisture Resistance of the Sensor

The stability of the CTL sensor using nano-SrO was investigated by detecting the CTL intensity of sevoflurane (SVF) three times a day for 7 day, as Figure S3A shows, the relative standard deviation (RSD) of the measured data is 3.6%, indicating the good stability of the sensor. Figure S3B shows that the humidity has no significant effect on the CTL detection, the RSD of CTL intensities measured under different humidity is 4.5%, which indicates the good moisture resistance of the sensor.

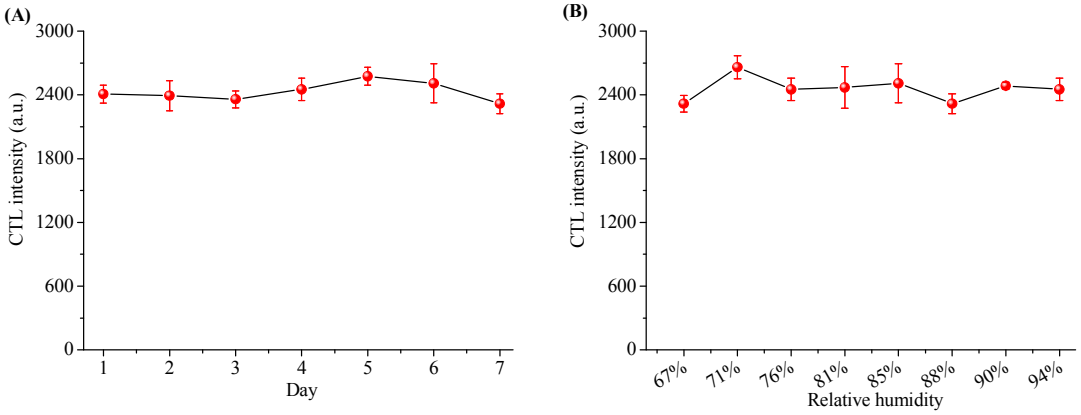

Figure S3. (A) The CTL intensities measured in 7 different days. (B) CTL intensities measured under different humidity**.** Working temperature, 210 °C; wavelength, 440 nm; flow rate, 400 mL/min (pressure = 74 hPa); concentrations of SVF, 15 μmoL/L.

4. The Transmission Electron Microscope Pattern of Nano-SrO

The transmission electron microscope (TEM) and X-ray power diffraction patterns of nano-SrO are shown in Figure S4A and Figure S4B, respectively. According to the standard X-ray power diffraction pattern (Powder Diffraction File: 06-0520), the phase of SrO was identified as cubic.

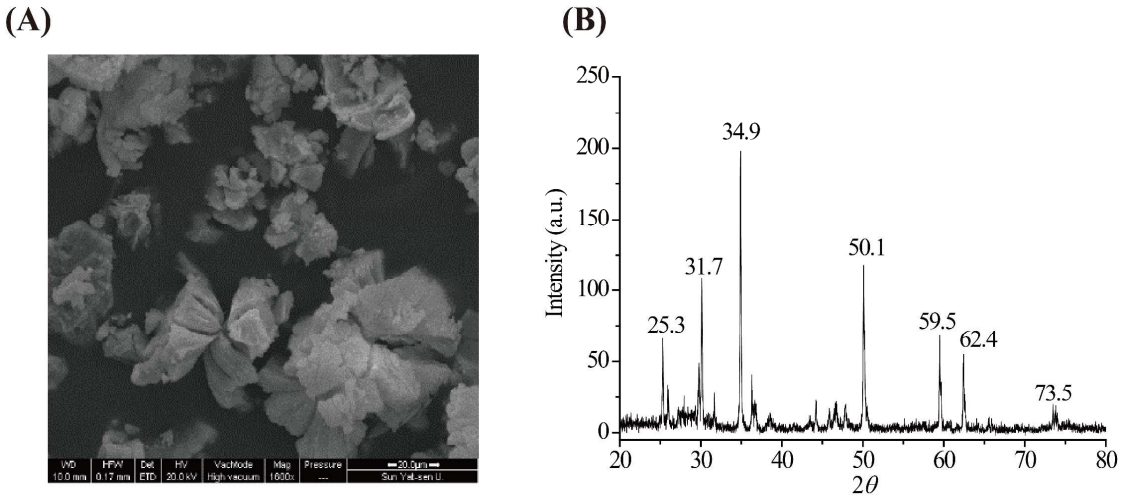

Figure S4. (A) The TEM pattern of nano-SrO. (B) The XRD pattern of nano-SrO.

5. The Influence of Reaction Conditions on CTL Analysis of Sevoflurane.

The influence of working temperature on CTL analysis of SVF is shown in Figure S5A. Working temperature at 210 ^{o}C was chosen as the optimum working temperature for CTL detection of SVF as the signal to noise ratio (SNR) was at its maximum at this temperature. The influence of detecting wavelength on CTL analysis of SVF is shown in Figure S5B. We chose 440 nm as the optimum detecting wavelength for CTL detection of SVF as the highest sensitivity at this detecting wavelength. The influence of flow rate on CTL intensity of SVF is shown in Figure S5C. It can be seen that the CTL intensity remain stable when flow rate over 150 mL/min, and 400 mL/min was chosen for the subsequent experiment.

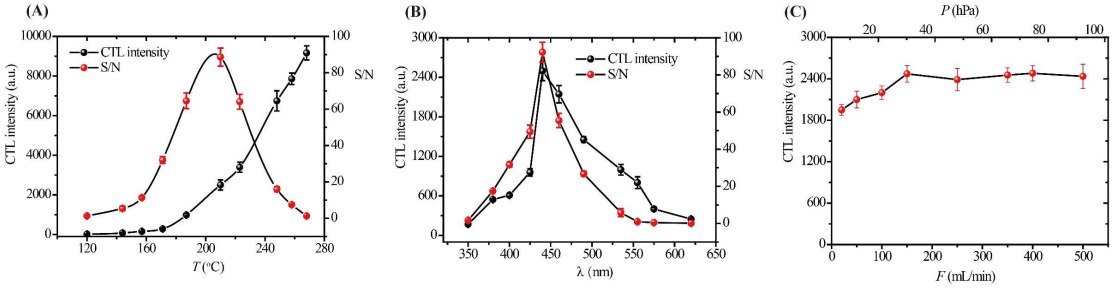

Figure S5. The influences of working conditions on CTL analysis of sevoflurane. (A) The influence of working temperature on CTL analysis of sevoflurane Wavelength, 440 nm; flow rate, 400 mL/min (pressure = 74 hPa); concentrations of SVF, 15 μmoL/L. (B) The influence of detecting wavelength on CTL analysis of sevoflurane. Working temperature, 210 °C; flow rate, 400 mL/min (pressure = 74 hPa); concentrations of sevoflurane, 15 μmoL/L. (C) The influence of flow rate on CTL analysis of sevoflurane. Working temperature, 210 °C; wavelength, 440 nm; concentrations of SVF, 15 μmoL/L.

6. The CTL Signals of the Limit of Detection and Blank Sample

During the experiment process, standard gaseous SVF samples were prepared by injecting certain microliter levels of liquid samples into the sampling bags, and clean air was used as diluents gas. No emissions were detected when clean air in sampling bag (blank sample) were the pumped into the CTL sensor, the measured results of SVF at concentration of 0.08 μmoL/L (detection limit of the present method) and blank sample are shown in Figure S6.

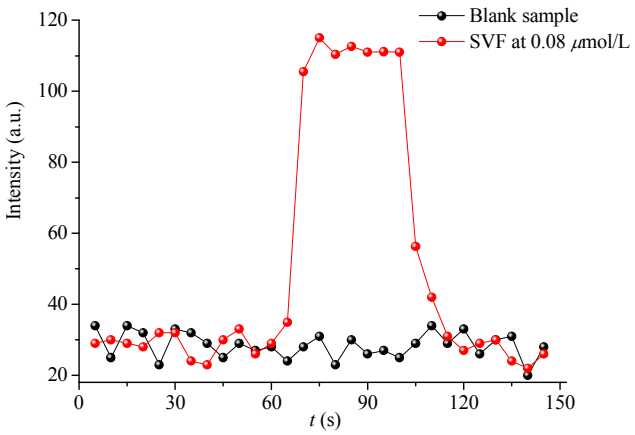

Figure 6. Measured results of SVF at concentration of 0.08 μmoL/L and blank sample. Working temperature, 210 °C; wavelength, 440 nm; flow rate, 400 mL/min (pressure = 74 hPa).

7. Comparison with Previously Reported Methods for Sevoflurane

The analytical characteristics of the present method were compared with the previously reported methods for SVF, as shown in Table S1.

Table S1. Comparison of the analytical methods for SVF

Method	Linear range (ppm)	LOD (ppm)	*r*	References
CTL sensor	4.5-1680	1.8	0.9933	Current method
GC-MS	0.33-33.21	*ND*	0.9997	1
GC-MS/MS	5.6-16800	1.0	0.9997	2
thermal desorption GC-MS	1.0×10^{-5}-1.0	5.0×10^{-6}	0.9990	3

ND stands for not discussion

8. The Representative CTL Intensity–Time Curves of the Four Groups of Rat Models

The representative CTL intensity–time curves of the four groups of rat models are shown in Figure S7.

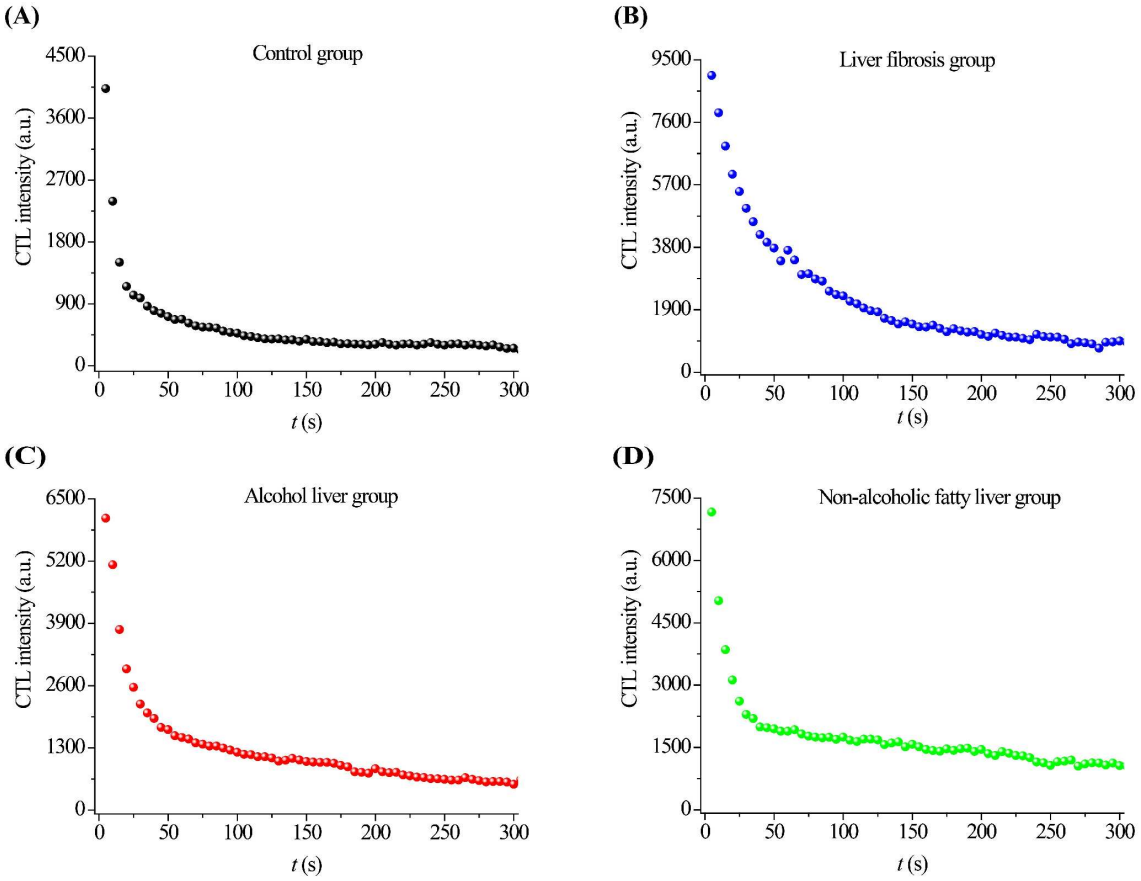

Figure S7. The representative CTL intensity–time curves the four groups of model animal. (A) Control group; (B) Liver fibrosis group; (C) Alcohol liver group; (D) Non-alcoholic fatty liver group. Working temperature, 210 °C; wavelength, 440 nm; flow rate, 400 mL/min (pressure = 74 hPa).

9. The Normalized Data of CTL Intensities for Linear Discriminate Analysis

The raw data of the CTL intensity–time curves of different groups were normalized and subsequently direct subjected to linear discriminate analysis (LDA), the normalized data of CTL intensities for LDA are listed in Table S2.

TableS2. The normalized data of CTL intensities for LDA

Group	Time (s)												
	0	5	10	15	20	25	30	35	40	45	50	55	60
Ⅰ(1)	1.00	0.63	0.46	0.39	0.35	0.32	0.31	0.30	0.29	0.28	0.28	0.26	0.23
Ⅰ(1)	1.00	0.49	0.32	0.25	0.21	0.18	0.16	0.15	0.14	0.13	0.12	0.11	0.10
Ⅰ(1)	1.00	0.60	0.44	0.36	0.33	0.31	0.29	0.29	0.30	0.27	0.28	0.27	0.26
Ⅰ(2)	1.00	0.63	0.44	0.35	0.30	0.28	0.27	0.23	0.25	0.24	0.23	0.22	0.22
Ⅰ(2)	1.00	0.54	0.41	0.35	0.32	0.31	0.30	0.28	0.27	0.26	0.27	0.25	0.23
Ⅰ(2)	1.00	0.59	0.40	0.28	0.23	0.20	0.18	0.19	0.19	0.18	0.17	0.17	0.17
Ⅰ(3)	1.00	0.63	0.43	0.34	0.28	0.26	0.25	0.24	0.23	0.22	0.22	0.20	0.20
Ⅰ(3)	1.00	0.59	0.47	0.36	0.31	0.31	0.32	0.31	0.32	0.27	0.27	0.27	0.24
Ⅰ(3)	1.00	0.59	0.37	0.29	0.26	0.24	0.22	0.20	0.19	0.18	0.17	0.17	0.15
Ⅱ(1)	1.00	0.76	0.61	0.54	0.47	0.41	0.41	0.38	0.32	0.28	0.27	0.24	0.23
Ⅱ(1)	1.00	0.84	0.73	0.60	0.51	0.44	0.39	0.34	0.33	0.31	0.29	0.27	0.26
Ⅱ(1)	1.00	0.82	0.69	0.59	0.52	0.47	0.43	0.40	0.36	0.34	0.32	0.30	0.28
Ⅱ(2)	1.00	0.73	0.60	0.51	0.45	0.40	0.37	0.36	0.34	0.32	0.31	0.28	0.27
Ⅱ(2)	1.00	0.80	0.69	0.59	0.50	0.47	0.45	0.44	0.42	0.42	0.39	0.38	0.37
Ⅱ(2)	1.00	0.78	0.67	0.59	0.54	0.51	0.49	0.47	0.46	0.42	0.40	0.45	0.39
Ⅱ(3)	1.00	0.75	0.62	0.55	0.49	0.45	0.43	0.39	0.37	0.35	0.33	0.32	0.33
Ⅱ(3)	1.00	0.82	0.67	0.60	0.54	0.49	0.45	0.43	0.41	0.38	0.38	0.39	0.39
Ⅱ(3)	1.00	0.77	0.66	0.55	0.47	0.42	0.40	0.37	0.33	0.32	0.30	0.30	0.28
Ⅲ(1)	1.00	0.75	0.60	0.54	0.51	0.46	0.48	0.47	0.46	0.45	0.46	0.45	0.47
Ⅲ(1)	1.00	0.75	0.60	0.48	0.48	0.42	0.41	0.42	0.41	0.36	0.36	0.36	0.35
Ⅲ(1)	1.00	0.74	0.59	0.50	0.45	0.41	0.38	0.35	0.33	0.32	0.31	0.30	0.29
Ⅲ(2)	1.00	0.74	0.58	0.50	0.43	0.40	0.37	0.34	0.33	0.30	0.30	0.29	0.27
Ⅲ(2)	1.00	0.76	0.62	0.53	0.46	0.41	0.37	0.34	0.32	0.31	0.29	0.28	0.27
Ⅲ(2)	1.00	0.73	0.57	0.47	0.39	0.34	0.31	0.27	0.26	0.27	0.27	0.26	0.24
Ⅲ(3)	1.00	0.76	0.61	0.51	0.46	0.41	0.38	0.35	0.33	0.32	0.30	0.29	0.30
Ⅲ(3)	1.00	0.74	0.62	0.53	0.49	0.47	0.41	0.40	0.41	0.41	0.42	0.45	0.41
Ⅲ(3)	1.00	0.73	0.57	0.51	0.44	0.39	0.34	0.33	0.31	0.26	0.23	0.22	0.20
Ⅲ(4)	1.00	0.75	0.67	0.58	0.56	0.53	0.49	0.47	0.44	0.42	0.40	0.39	0.37
Ⅲ(4)	1.00	0.72	0.62	0.59	0.52	0.52	0.49	0.52	0.50	0.50	0.47	0.50	0.49
Ⅲ(4)	1.00	0.73	0.58	0.52	0.47	0.43	0.41	0.39	0.40	0.36	0.35	0.36	0.33

Ⅳ(1)	1.00	0.70	0.51	0.42	0.35	0.28	0.25	0.23	0.20	0.19	0.17	0.16	0.15
Ⅳ(1)	1.00	0.69	0.49	0.41	0.38	0.37	0.33	0.31	0.32	0.31	0.30	0.30	0.29
Ⅳ(1)	1.00	0.64	0.48	0.35	0.29	0.26	0.24	0.23	0.22	0.21	0.21	0.21	0.20
Ⅳ(2)	1.00	0.69	0.47	0.38	0.31	0.28	0.27	0.25	0.23	0.23	0.22	0.21	0.21
Ⅳ(2)	1.00	0.69	0.51	0.39	0.32	0.29	0.26	0.22	0.21	0.20	0.20	0.19	0.18
Ⅳ(2)	1.00	0.70	0.51	0.42	0.35	0.28	0.25	0.23	0.20	0.19	0.17	0.16	0.15
Ⅳ(3)	1.00	0.70	0.54	0.44	0.36	0.32	0.31	0.28	0.28	0.27	0.26	0.26	0.27
Ⅳ(3)	1.00	0.68	0.55	0.46	0.42	0.38	0.36	0.33	0.32	0.29	0.29	0.27	0.27
Ⅳ(3)	1.00	0.68	0.50	0.37	0.29	0.23	0.20	0.17	0.17	0.17	0.15	0.14	0.13
Ⅲ(4)	1.00	0.71	0.54	0.44	0.35	0.31	0.28	0.26	0.24	0.23	0.22	0.22	0.22
Ⅳ(4)	1.00	0.70	0.51	0.42	0.35	0.28	0.25	0.23	0.20	0.19	0.17	0.16	0.15
Ⅳ(4)	1.00	0.70	0.51	0.38	0.28	0.23	0.20	0.18	0.17	0.15	0.15	0.14	0.13

Group	Time (s)												
	65	70	75	80	85	90	95	100	105	110	115	120	125
Ⅰ(1)	0.21	0.24	0.24	0.24	0.24	0.22	0.21	0.17	0.17	0.17	0.18	0.18	0.17
Ⅰ(1)	0.10	0.09	0.09	0.09	0.08	0.07	0.08	0.07	0.08	0.08	0.07	0.08	0.07
Ⅰ(1)	0.27	0.25	0.25	0.25	0.23	0.22	0.21	0.22	0.21	0.21	0.21	0.20	0.21
Ⅰ(2)	0.21	0.20	0.22	0.20	0.20	0.19	0.19	0.19	0.16	0.19	0.18	0.18	0.17
Ⅰ(2)	0.24	0.23	0.22	0.22	0.21	0.21	0.22	0.21	0.20	0.19	0.19	0.19	0.19
Ⅰ(2)	0.16	0.15	0.15	0.15	0.14	0.14	0.14	0.13	0.13	0.13	0.12	0.13	0.12
Ⅰ(3)	0.19	0.19	0.19	0.18	0.18	0.17	0.17	0.17	0.16	0.15	0.15	0.15	0.14
Ⅰ(3)	0.24	0.24	0.24	0.25	0.23	0.21	0.21	0.19	0.19	0.21	0.19	0.21	0.18
Ⅰ(3)	0.14	0.14	0.14	0.14	0.12	0.12	0.12	0.11	0.11	0.10	0.10	0.10	0.10
Ⅱ(1)	0.23	0.20	0.20	0.20	0.20	0.18	0.18	0.17	0.16	0.17	0.16	0.16	0.16
Ⅱ(1)	0.25	0.23	0.24	0.22	0.21	0.23	0.22	0.22	0.21	0.22	0.21	0.21	0.21
Ⅱ(1)	0.32	0.28	0.26	0.25	0.24	0.23	0.23	0.23	0.23	0.22	0.23	0.22	0.21
Ⅱ(2)	0.26	0.26	0.25	0.25	0.25	0.24	0.23	0.23	0.24	0.23	0.22	0.22	0.21
Ⅱ(2)	0.36	0.34	0.33	0.32	0.33	0.30	0.31	0.32	0.30	0.30	0.30	0.30	0.30
Ⅱ(2)	0.35	0.36	0.35	0.35	0.36	0.35	0.35	0.33	0.35	0.34	0.33	0.35	0.16
Ⅱ(3)	0.31	0.30	0.30	0.29	0.30	0.30	0.30	0.28	0.28	0.28	0.29	0.30	0.32
Ⅱ(3)	0.40	0.41	0.41	0.44	0.46	0.46	0.42	0.44	0.44	0.42	0.41	0.38	0.37
Ⅱ(3)	0.28	0.25	0.25	0.24	0.25	0.22	0.23	0.23	0.22	0.22	0.22	0.22	0.27
Ⅲ(1)	0.45	0.47	0.43	0.45	0.42	0.45	0.44	0.43	0.39	0.43	0.45	0.44	0.39
Ⅲ(1)	0.37	0.33	0.38	0.34	0.35	0.32	0.33	0.31	0.33	0.32	0.35	0.26	0.32
Ⅲ(1)	0.28	0.25	0.25	0.24	0.24	0.26	0.22	0.18	0.20	0.20	0.18	0.15	0.13
Ⅲ(2)	0.27	0.26	0.26	0.25	0.24	0.24	0.23	0.23	0.22	0.22	0.21	0.20	0.20
Ⅲ(2)	0.27	0.26	0.24	0.23	0.23	0.22	0.22	0.21	0.21	0.20	0.20	0.20	0.19
Ⅲ(2)	0.18	0.20	0.19	0.16	0.18	0.15	0.15	0.12	0.16	0.17	0.16	0.15	0.14
Ⅲ(3)	0.30	0.31	0.31	0.29	0.28	0.26	0.25	0.25	0.24	0.24	0.24	0.20	0.21
Ⅲ(3)	0.40	0.36	0.35	0.29	0.40	0.39	0.35	0.38	0.35	0.30	0.32	0.28	0.22
Ⅲ(3)	0.24	0.27	0.25	0.19	0.20	0.14	0.17	0.19	0.20	0.22	0.21	0.21	0.18
Ⅲ(4)	0.34	0.35	0.33	0.32	0.30	0.26	0.25	0.21	0.22	0.21	0.18	0.19	0.20

Ⅲ(4)	0.50	0.40	0.48	0.51	0.44	0.39	0.37	0.36	0.37	0.38	0.38	0.38	0.37
Ⅲ(4)	0.32	0.32	0.31	0.30	0.31	0.32	0.31	0.30	0.31	0.29	0.29	0.30	0.30
Ⅳ(1)	0.14	0.15	0.14	0.14	0.13	0.12	0.12	0.11	0.11	0.11	0.11	0.12	0.12
Ⅳ(1)	0.30	0.30	0.29	0.28	0.27	0.29	0.30	0.26	0.31	0.32	0.30	0.30	0.31
Ⅳ(1)	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.18	0.18	0.17	0.16
Ⅳ(2)	0.20	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.18	0.18	0.18	0.18	0.17
Ⅳ(2)	0.17	0.17	0.16	0.15	0.15	0.14	0.14	0.15	0.13	0.13	0.13	0.13	0.13
Ⅳ(2)	0.14	0.15	0.14	0.14	0.13	0.12	0.12	0.11	0.11	0.11	0.11	0.12	0.12
Ⅳ(3)	0.25	0.25	0.24	0.24	0.24	0.24	0.24	0.23	0.23	0.24	0.24	0.23	0.22
Ⅳ(3)	0.26	0.25	0.24	0.23	0.22	0.22	0.22	0.20	0.20	0.18	0.18	0.20	0.20
Ⅳ(3)	0.13	0.12	0.11	0.11	0.10	0.10	0.09	0.09	0.08	0.08	0.09	0.10	0.10
Ⅳ(4)	0.21	0.21	0.20	0.20	0.19	0.19	0.19	0.19	0.18	0.19	0.17	0.17	0.17
Ⅳ(4)	0.14	0.15	0.14	0.14	0.13	0.12	0.12	0.11	0.11	0.11	0.11	0.12	0.12
Ⅳ(4)	0.13	0.12	0.12	0.12	0.11	0.11	0.11	0.11	0.10	0.10	0.10	0.10	0.10

1. Ⅰ, Ⅱ, Ⅲ, Ⅳ stand for rat models of control group (*n*=3), liver fibrosis group (*n*=3), alcohol liver group (*n*=4) and non-alcoholic fatty liver group (*n*=4).
2. The Arabic numerals (1, 2, 3, 4) marked behind the groups of rat models stand for different individuals of the group.

10. 2D Canonical Score Plots of the CTL Intensity–Time Curves on Three Different Days Analyzed by LDA Independently

The 2D canonical score plots of the CTL intensity–time curves on three different days analyzed by LDA independently are shown in Figure S8.

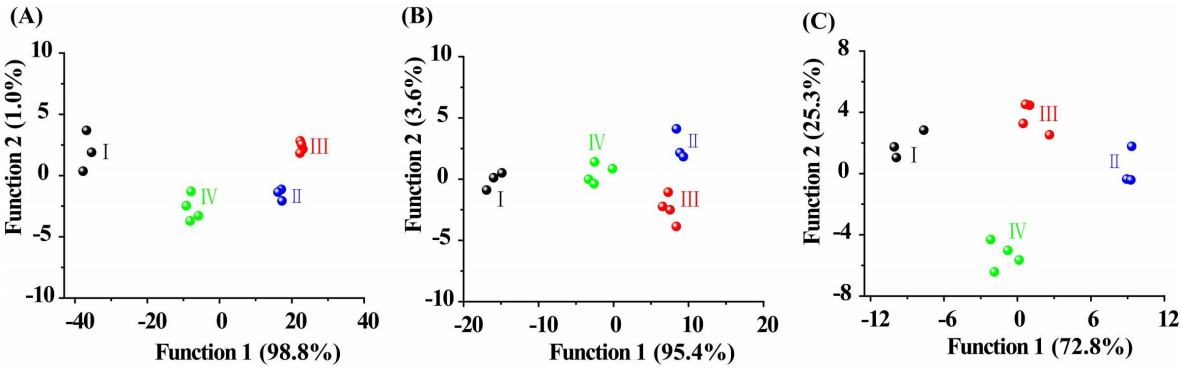

Figure S8. The 2D canonical score plots of the CTL intensity–time curves on three different days analyzed by LDA independently.

11. Results of One-Way Analysis of Variance

The normalized data of CTL intensities listed in Table S2 were analyzed by one-way analysis of variance. As Table S3 shows, the *p*-values of overwhelming majority of data are greater than 0.05 (only 6 in 500 *p*-values are less than 0.05), indicating that there is no significant statistical difference between the replicates conducted in three different days.

Table S3. Results of one-way analysis of variance

Group	Time (s)	Sum of square	Df	Mean square	*F*	*P*
I	5	0.012	2.000	0.006	7.276	0.025
	10	0.003	2.000	0.002	0.730	0.520
	15	0.004	2.000	0.002	1.000	0.422
	20	0.002	2.000	0.001	0.450	0.658
	25	0.002	2.000	0.001	0.314	0.742
	30	0.003	2.000	0.002	0.433	0.668
	35	0.001	2.000	0.001	0.179	0.840
	40	0.001	2.000	0.001	0.150	0.864
	45	0.002	2.000	0.001	0.332	0.730
	50	0.002	2.000	0.001	0.247	0.789
	55	0.001	2.000	0.000	0.110	0.898
	60	0.001	2.000	0.001	0.195	0.828
	65	0.000	2.000	0.000	0.037	0.963
	70	0.001	2.000	0.001	0.195	0.828
	75	0.002	2.000	0.001	0.337	0.726
	80	0.001	2.000	0.001	0.146	0.867
	85	0.003	2.000	0.002	0.421	0.674
	90	0.002	2.000	0.001	0.304	0.748
	95	0.002	2.000	0.001	0.290	0.758
	100	0.001	2.000	0.000	0.154	0.860
	105	0.000	2.000	0.000	0.055	0.947
	110	0.001	2.000	0.000	0.145	0.868
	115	0.001	2.000	0.001	0.203	0.822
	120	0.001	2.000	0.001	0.209	0.817
	125	0.000	2.000	0.000	0.086	0.919
II	5	0.008	2.000	0.004	9.175	0.015
	10	0.012	2.000	0.006	14.289	0.005
	15	0.006	2.000	0.003	9.433	0.014
	20	0.004	2.000	0.002	2.688	0.147
	25	0.004	2.000	0.002	1.941	0.224
	30	0.002	2.000	0.001	0.764	0.506
	35	0.002	2.000	0.001	0.548	0.605

	40	0.003	2.000	0.002	0.680	0.542
	45	0.005	2.000	0.002	1.014	0.417
	50	0.004	2.000	0.002	0.892	0.458
	55	0.009	2.000	0.005	1.037	0.410
	60	0.006	2.000	0.003	0.805	0.490
	65	0.008	2.000	0.004	1.315	0.336
	70	0.008	2.000	0.004	0.874	0.464
	75	0.009	2.000	0.004	1.037	0.411
	80	0.010	2.000	0.005	0.813	0.487
	85	0.011	2.000	0.005	0.702	0.532
	90	0.013	2.000	0.006	0.846	0.475
	95	0.010	2.000	0.005	0.787	0.497
	100	0.015	2.000	0.008	1.245	0.353
	105	0.012	2.000	0.006	0.817	0.486
	110	0.011	2.000	0.006	0.957	0.436
	115	0.010	2.000	0.005	0.874	0.464
	120	0.007	2.000	0.004	0.620	0.569
	125	0.011	2.000	0.005	0.992	0.424
III	5	0.001	2.000	0.000	2.413	0.145
	10	0.004	2.000	0.002	3.325	0.083
	15	0.003	2.000	0.001	1.117	0.369
	20	0.007	2.000	0.004	2.084	0.180
	25	0.010	2.000	0.005	1.907	0.204
	30	0.011	2.000	0.006	2.016	0.189
	35	0.017	2.000	0.008	1.897	0.205
	40	0.016	2.000	0.008	1.738	0.230
	45	0.019	2.000	0.009	1.973	0.195
	50	0.020	2.000	0.010	2.016	0.189
	55	0.026	2.000	0.013	2.007	0.190
	60	0.029	2.000	0.014	2.187	0.168
	65	0.035	2.000	0.017	2.792	0.114
	70	0.018	2.000	0.009	1.968	0.195
	75	0.027	2.000	0.014	2.361	0.150
	80	0.034	2.000	0.017	1.993	0.192
	85	0.031	2.000	0.015	2.619	0.127
	90	0.028	2.000	0.014	1.731	0.231
	95	0.024	2.000	0.012	1.866	0.210
	100	0.029	2.000	0.015	2.017	0.189
	105	0.019	2.000	0.010	1.774	0.224
	110	0.013	2.000	0.007	1.056	0.387
	115	0.021	2.000	0.011	1.299	0.319
	120	0.013	2.000	0.006	0.750	0.500
	125	0.016	2.000	0.008	1.112	0.370
IV	5	0.001	2.000	0.000	1.286	0.323

10	0.001	2.000	0.000	0.466	0.642
15	0.004	2.000	0.002	2.526	0.135
20	0.009	2.000	0.004	3.860	0.062
25	0.013	2.000	0.006	5.169	0.032
30	0.013	2.000	0.006	4.560	0.043
35	0.011	2.000	0.005	3.500	0.075
40	0.011	2.000	0.005	2.661	0.124
45	0.010	2.000	0.005	2.681	0.122
50	0.010	2.000	0.005	2.410	0.145
55	0.010	2.000	0.005	2.069	0.182
60	0.011	2.000	0.006	2.113	0.177
65	0.011	2.000	0.005	1.870	0.209
70	0.011	2.000	0.006	2.223	0.164
75	0.010	2.000	0.005	1.920	0.202
80	0.009	2.000	0.004	1.727	0.232
85	0.009	2.000	0.004	1.703	0.236
90	0.009	2.000	0.005	1.371	0.302
95	0.011	2.000	0.005	1.436	0.288
100	0.008	2.000	0.004	1.391	0.298
105	0.010	2.000	0.005	1.197	0.346
110	0.011	2.000	0.006	1.237	0.335
115	0.009	2.000	0.004	1.130	0.365
120	0.010	2.000	0.005	1.425	0.290
125	0.010	2.000	0.005	1.539	0.266

* Ⅰ, Ⅱ, Ⅲ, Ⅳ stand for rat models of control group (n=3), liver fibrosis group (n=3), alcohol liver group (n=4) and non-alcoholic fatty liver group (n=4).

12. The Detailed Parameters for Linear Discriminate Analysis of 42 Data Sets.

The detailed parameters for LDA of 42 data sets (14 rat models × 3 assays) are shown in Table S4 and Table S5.

Table S4. Test of equality of group means

Variable	Wilks' Lambda	F	Df_1	Df_2	*P*
0	-	-	-	-	-
5	0.154	69.761	3	38	0.000
10	0.129	85.598	3	38	0.000
15	0.134	82.172	3	38	0.000
20	0.185	55.871	3	38	0.000
25	0.269	34.364	3	38	0.000
30	0.295	30.262	3	38	0.000
35	0.345	24.099	3	38	0.000
40	0.434	16.532	3	38	0.000
45	0.431	16.694	3	38	0.000
50	0.470	14.292	3	38	0.000
55	0.502	12.588	3	38	0.000
60	0.517	11.855	3	38	0.000
65	0.518	11.779	3	38	0.000
70	0.540	10.783	3	38	0.000
75	0.541	10.738	3	38	0.000
80	0.630	7.446	3	38	0.000
85	0.581	9.132	3	38	0.000
90	0.641	7.096	3	38	0.001
95	0.643	7.041	3	38	0.001
100	0.655	6.664	3	38	0.001
105	0.622	7.689	3	38	0.000
110	0.632	7.390	3	38	0.001
115	0.645	6.967	3	38	0.001
120	0.675	6.097	3	38	0.002
125	0.708	5.214	3	38	0.004

Table S5. Eigenvalues

Function	Eigenvalue	% of Variance	Cumulative %	Canonical Correlation
1	47.016[a]	78.6	78.6	0.990
2	11.191[a]	18.7	97.3	0.958
3	1.626[a]	2.7	100.0	0.787

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