Point-of-care detection of sevoflurane anesthetics in exhaled breath using miniature TOFMS for diagnosis of postoperative agitation symptoms in children

Bing Liu[†,#], Wenxi Tang[§,#], Hang Li[‡], Ruidong Liu[†], Fengshuo Dong[†], Yingzhe Guo[†], Jianjun Li [§] and Keyong Hou [*,†]

[†]Environment Research Institute, Shandong University, 72 Binhai Road, Qingdao 266237, People's Republic of China

[§]Department of Anesthesiology, Qilu Hospital (Qingdao), Cheeloo College of Medicine, Shandong University, Qingdao, 758 Hefei Road, Qingdao 266035, People's Republic of China

[‡]Key Laboratory of Separation Science for Analytical Chemistry, Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Dalian 116023, People's Republic of China

*Corresponding Author

E-mail: houky@sdu.edu.cn;

Tel: +86-0532-58631956;

This supporting material includes additional information on the following aspects:

The exhaled respiratory simulation system is shown in Figure S1. It consisted of compressed air a glass flask and water bath. The compressed air was mixed with CO_2 in proportion by mass flow controller to simulate the real exhaled air. The flow of the mixed gas was controlled at 0.91 mL/min. The water bath was adjusted to 38 °C, and the simulated mixed gas was passed into a flask containing water at 38 degrees Celsius, and the relative humidity of the simulated exhaled gas was 88.4% , which measured by a dew point detector.

Fig. S1 Device diagram of exhalation simulation system.

As shown in Figure S2, for the exhaled gas spectrum of healthy people, we can detected H_2O, CO_2, N_2 and O_2 in the exhaled gas, and found that there was no background peak at M / Z = 181.

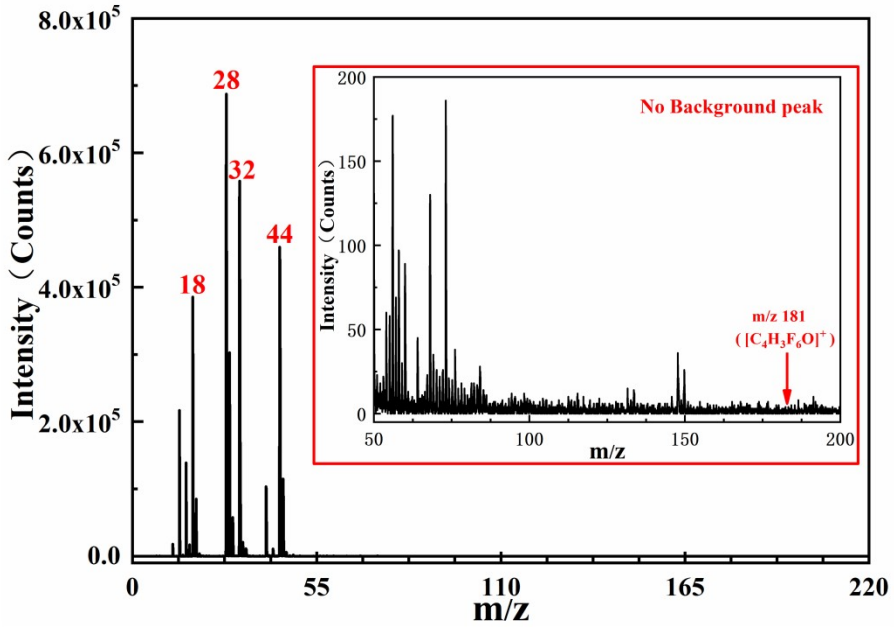

Fig. S2 Spectrum of exhaled gas from healthy people obtained with the miniature MEPEI -TOFMS.

As shown in Figure S3, it was a picture of the application of miniature TOFMS in the hospital. Figure S3a showed the picture of real-time monitoring of patients' exhalation during operation, Figure S3b showed the picture of environment of medical places and exhalation pipeline, Figure S3c showed the picture of resuscitation room and Figure S3d showed the picture of real-time monitoring of patients' exhalation in the resuscitation room.

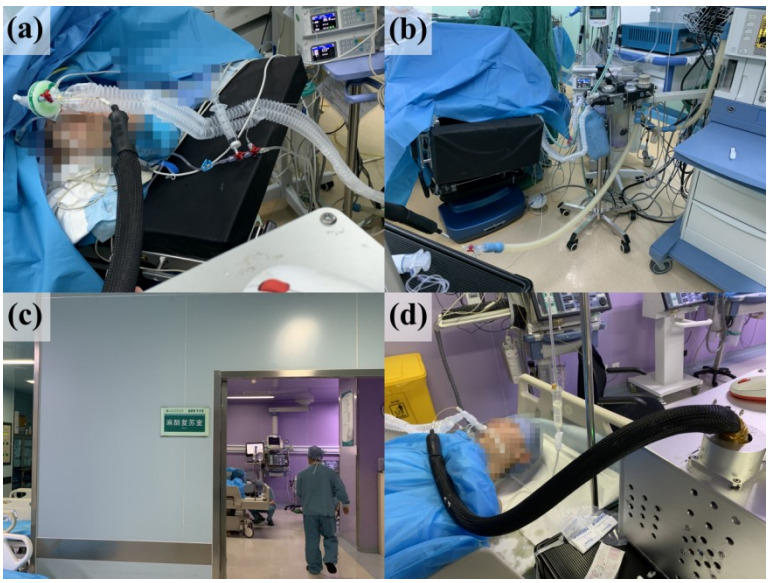

Fig. S3 Pictures of (a) Real-time monitoring of patients' exhalation during operation, (b) Environment of medical places and exhalation pipeline, (c) Resuscitation room and (d) Real-time monitoring of patients' exhalation in the resuscitation room.

As shown in Table S1, we recorded restless patients' gender, age, height, weight, type of operation and so on. All patients were preschool and school-age children aged 2-12 years with standard height, weight and no family history of genetic diseases. In addition, the use of nerve blockers was recorded, which determined whether the patient had pain during the recovery period. The awakening concentrations of four restless patients were 1339 ppmv, 992 ppmv, 563 ppmv, 550 ppmv and the awakening time was 4 min, 11 min, 10 min and 4 min respectively.

Table S1 The basic information of restless patients.

Number	Type of surgery	Pain	Gender	Age	Height/cm	Weight/kg	Awakening concentration/ppmv	Awakening time/min
a	Orthopaedics	No	Male	10	150	25	1339	4

b	Orthopaedics	No	Female	8	135	30	992	11
c	Orthopaedics	No	Female	9	140	24.5	563	10
d	Orthopaedics	No	Male	3	107	25	550	4

As shown in Figure S4, the intercept of R^2 on the Y axis was -0.0663 (less than 0.4) and the intercept of Q^2 on the Y axis was -0.12 (less than 0.05) in the validate model curve. The results showed that the model had no over-fitting, the interpretation ability and prediction ability of the model were great.

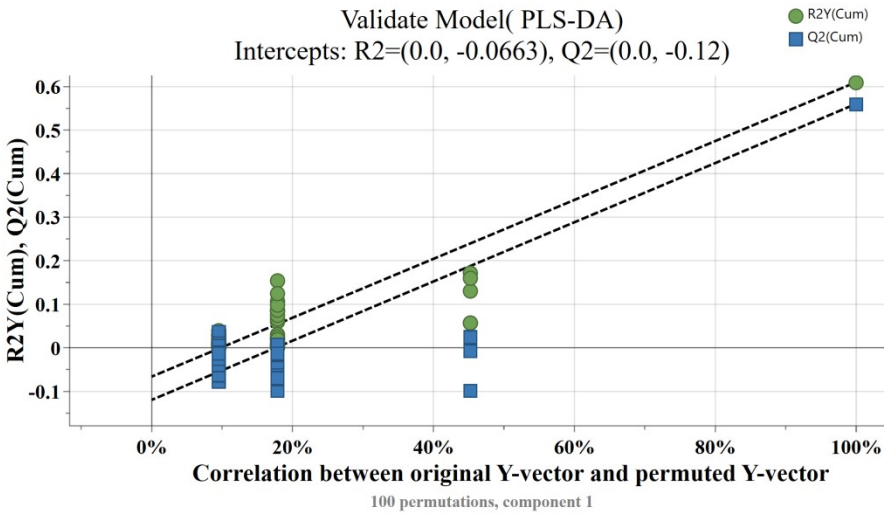

Fig. S4 The validate model curve obtained by analyzing the fitted data of all cases.