

The selection criteria for PD patients

1. Women during the premenstrual or menstrual period mainly presented cyclical abdominal pain syndrome accompanied with other discomforts, thereby affecting their work and lives.
2. Gynecological examination showed no organic genital lesions.
3. Patients' ages ranged from 16 to 35 years old.
4. Patients had regular menstrual cycles of 21–35 d.
5. Prior to this study, dysmenorrhea patients neither received other methods of treatment during their menstrual cycle, nor did they take painkillers, sedatives, or steroids.
6. A dysmenorrhea integral over 8 indicated pain.

Table S1. Dysmenorrhea integral

Symptoms	points
Abdominal pain before and after menstruation	5 (basis points)
Unbearable abdominal pain	1
Abdominal pain obviously	0.5
Feel restless	1
Of shock	2
Paleness	0.5
Cold sweat and delightfully	1
Limbs jueleng	1
Require to stay in bed	1
Affect the work learning	1
Do not relieve pain with the general measures	1
Suspension with general measures of analgesic pain	0.5
With lower back pain	0.5
With nausea and vomiting	0.5
With anal bulge	0.5
Pain in less than one day	0.5
Each additional day of pain	0.5

Note: mild, dysmenorrhea symptom score of <8 points; moderate, dysmenorrhea symptom score from 8 to 12 points; and severe, dysmenorrhea symptom score of >12 points.

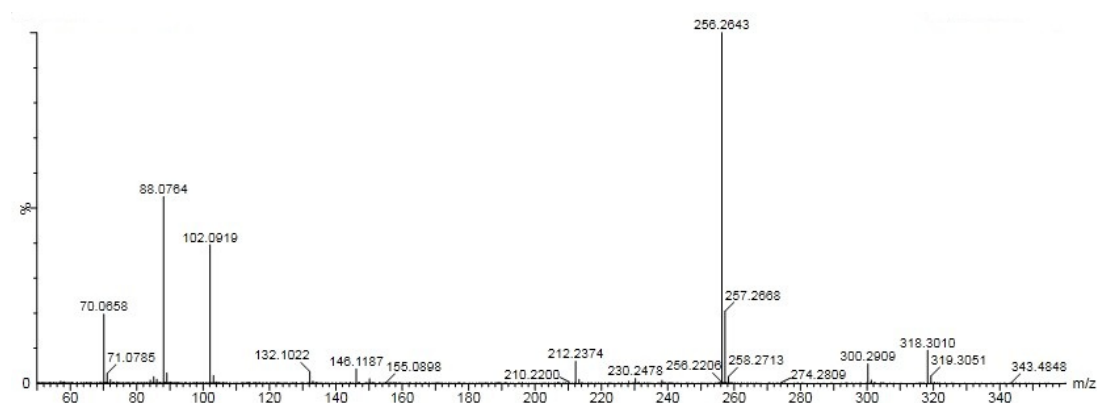
Table S2. R² and Q² value of established PLS-DA models.

Primary dysmenorrhea vs healthy volunteers	
R ² Y	1.000
R ² X	0.239
Q ²	0.688

Note: R² and Q² parameters indicate the fitness and prediction of the model.

Table S3: The different in RT of the identified metabolites with five standards

No.	Rt(min)	RT(standards)	△RT(s)	compound
1	0.85	0.78	4.20	Threonine
2	0.76	0.70	3.60	Lysine
3	2.67	2.59	4.80	Phenylalanine
4	1.60	1.68	-4.80	Tyrosine
5	12.35	12.28	4.20	17-Hydroxyprogesterone

Fig S1. The identification of phytosphingosine (t_R=12.18min, m/z=318.3010).

According to the retention time of the corresponding peak from the total ion chromatogram, the exact mass of markers was 318.3010. By searching the HMDB database, the molecular formula was obtained for phytosphingosine. In the positive

ion model, the main fragment ions in the MS/MS spectrum contain 256.2 $[M+H-C_2H_5O_2]^+$ and 146.1 $[M+H-C_{11}H_{23}O]^+$. Relevant literature data were consulted to confirm the structure of this ion, and this metabolite was inferred to be phytosphingosine.