Supporting Information

Determination of active ingredients in Chinese medicine Danning Tablets using dispersion solid-phase extraction by molecular imprinting nanomaterials coupled with HPLC-DAD

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1. Peak purity calculation method

Peak purity is a measure of whether a chromatographic peak detected by a photodiode array detector contains multiple components. The LabSolutions workstation of Shimadzu calculates the similarity of the object spectrum and the reference spectrum. The similarity is compared with the threshold obtained from the noise component calculation to determine the peak purity.

1.1 Similarity calculation

Similarity is a measure of the matching of two spectra (object spectrum and reference spectrum). The spectrum was used as the absorbance at each wavelength and the absorption

spectra $\mathbf{S_1}$ and $\mathbf{S_2}$ were represented by the following vectors, where (λ_1) represents the absorbance at the wavelength (λ_1):

$\mathbf{S_1} = (\mathbf{a_1}(\lambda_1), \mathbf{a_1}(\lambda_2), \ldots, \mathbf{a_1}(\lambda_n))$,

$\mathbf{S_2} = (\mathbf{a_2}(\lambda_1), \mathbf{a_2}(\lambda_2), \ldots, \mathbf{a_2}(\lambda_n))$

The smaller the angle θ formed between $\mathbf{S_1}$ and $\mathbf{S_2}$, the greater the similarity of the two spectra. The similarity ($\mathbf{S_I}$) of two spectra was obtained by calculating $\cos\theta$ with the following equation:

$$\mathbf{S_I} = \frac{\mathbf{S_1} \bullet \mathbf{S_2}}{|\mathbf{S_1}||\mathbf{S_2}|} = \cos\theta, \quad |\mathbf{S_1}| = \sqrt{\sum \mathbf{a_1}(\lambda_i)^2}, \quad |\mathbf{S_2}| = \sqrt{\sum \mathbf{a_2}(\lambda_i)^2}$$

The $\mathbf{S_I}$ is closer to 1, indicating that the object spectrum and the reference spectrum matched more satisfactorily.

1.2 Threshold calculation

Due to background noise of the detector, absorption noise of mobile phase and other factors, the angle θ between $\mathbf{S_1}$ and $\mathbf{S_2}$ may change. The circle with radius N represents the uncertainty caused by noise component of various sizes N. The $\cos(\theta_1 + \theta_2)$ produced by noise could reduce the similarity of object spectrum and reference spectrum. However, if the θ between two spectra was greater than (θ_1 + θ_2), there were other factors that caused the two spectra to have different shapes except noise component. $\cos(\theta_1 + \theta_2)$ is referred to threshold (t) computed by Eq. (1), the noise spectral intensity at the wavelength λ_i is assumed as $no(\lambda_i)$, so N is expressed by Eq. (2):

$$t = \cos(\theta_1 + \theta_2) = \sqrt{\left(1 - \frac{N^2}{|\mathbf{S_1}|^2}\right) \times \left(1 - \frac{N^2}{|\mathbf{S_2}|^2}\right)} - \frac{N^2}{|\mathbf{S_1}||\mathbf{S_2}|} \qquad (1)$$

$$N = \sqrt{\sum no(\lambda_i)^2} \qquad (2)$$

1.3 Peak purity calculation

Peak purity index (*PPI*) was obtained through the difference between similarity and threshold

with the following equation:

$$PPI = (\boldsymbol{S_I} - t) \times 10^6$$

As listed in Table S1, *PPI* was used to determine the peak purity.

The above is the reference to LabSolutions workstation theoretical manual (223-60090, Revision C March 2012) of Shimadzu.

Table S1 Purity judgment

$S_I \geq t$	$PPI \geq 0$	pure
$S_I < t$	$PPI < 0$	impure