

表 S1 星点设计因素与水平

Table S1 Factors and levels of central composite design (CCD)

| Factor | Levels |      |      |      |      |
|--------|--------|------|------|------|------|
|        | -1.68  | -1   | 0    | 1    | 1.68 |
| $X_1$  | 0.03   | 0.10 | 0.20 | 0.30 | 0.37 |
| $X_2$  | 4.92   | 5.60 | 6.60 | 7.60 | 8.28 |
| $X_3$  | 0.46   | 0.60 | 0.80 | 1.00 | 1.14 |

$X_1$ : w (sodium dodecyl sulfate (SDS))/%;  $X_2$ : w (n-butanol)/%;  $X_3$ : w (cyclohexane)/%.

表 S2 星点设计实验安排与结果

Table S2 Experimental designs and results of CCD

| No. | $X_1$ | $X_2$ | $X_3$ | COF     |
|-----|-------|-------|-------|---------|
| 1   | 0.10  | 5.60  | 0.60  | 5.932   |
| 2   | 0.30  | 5.60  | 0.60  | -0.080  |
| 3   | 0.10  | 7.60  | 0.60  | 1.893   |
| 4   | 0.30  | 7.60  | 0.60  | -2.288  |
| 5   | 0.10  | 5.60  | 1.00  | -8.216  |
| 6   | 0.30  | 5.60  | 1.00  | -12.937 |
| 7   | 0.10  | 7.60  | 1.00  | -1.211  |
| 8   | 0.30  | 7.60  | 1.00  | 0.182   |
| 9   | 0.03  | 6.60  | 0.80  | -3.953  |
| 10  | 0.37  | 6.60  | 0.80  | -7.601  |
| 11  | 0.20  | 4.92  | 0.80  | -8.253  |
| 12  | 0.20  | 8.28  | 0.80  | -1.704  |
| 13  | 0.20  | 6.60  | 0.46  | 3.955   |
| 14  | 0.20  | 6.60  | 1.14  | -2.846  |
| 15  | 0.20  | 6.60  | 0.80  | 3.029   |
| 16  | 0.20  | 6.60  | 0.80  | 3.050   |
| 17  | 0.20  | 6.60  | 0.80  | 3.108   |
| 18  | 0.20  | 6.60  | 0.80  | 3.123   |

|    |      |      |      |       |
|----|------|------|------|-------|
| 19 | 0.20 | 6.60 | 0.80 | 3.138 |
| 20 | 0.20 | 6.60 | 0.80 | 3.109 |

$X_1, X_2, X_3$  are the same as in Table S1. COF: overall desirability function.

**表S3** 星点设计实验10种药物的分离度( $R$ )及分离时间

**Table S3** Resolutions ( $R$ ) and separation times of the 10 drugs by CCD

| No. | $R_{1,2}$ | $R_{2,3}$ | $R_{3,4}$ | $R_{4,5}$ | $R_{5,6}$ | $R_{6,7}$ | $R_{7,8}$ | $R_{8,9}$ | $R_{9,10}$ | $T_L$ |
|-----|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|------------|-------|
| 1   | 4.31      | 2.33      | 3.11      | 2.09      | 3.01      | 1.79      | 3.63      | 1.05      | 2.25       | 27.44 |
| 2   | 2.23      | 8.28      | 2.49      | 0.73      | 2.38      | 2.09      | 1.47      | 2.03      | 1.09       | 30.35 |
| 3   | 3.97      | 1.24      | 2.68      | 4.65      | 0.62      | 1.89      | 3.28      | 0.28      | 1.89       | 22.30 |
| 4   | 2.53      | 6.80      | 2.97      | 1.19      | 0.08      | 3.74      | 1.19      | 2.98      | 0.25       | 22.96 |
| 5   | 2.22      | 0.74      | 2.46      | 1.04      | 2.82      | 0.46      | 3.86      | 0.66      | 1.91       | 18.35 |
| 6   | 1.52      | 5.46      | 2.62      | 0.02      | 1.58      | 2.71      | 0.15      | 3.03      | 0.22       | 20.44 |
| 7   | 3.66      | 1.10      | 2.73      | 0.78      | 2.80      | 2.85      | 4.23      | 0.88      | 2.28       | 19.22 |
| 8   | 2.05      | 5.89      | 2.08      | 0.74      | 1.32      | 1.98      | 2.30      | 1.95      | 0.60       | 18.92 |
| 9   | 2.05      | 2.07      | 0.73      | 0.06      | 1.39      | 5.94      | 4.89      | 0.49      | 3.42       | 22.55 |
| 10  | 1.76      | 7.34      | 2.68      | 0.35      | 1.46      | 3.30      | 0.05      | 3.40      | 0.31       | 23.28 |
| 11  | 2.79      | 4.73      | 3.95      | 0.01      | 1.87      | 3.32      | 0.21      | 2.53      | 0.06       | 24.69 |
| 12  | 2.59      | 3.63      | 2.00      | 0.27      | 3.13      | 0.30      | 3.87      | 1.63      | 1.20       | 18.20 |
| 13  | 3.87      | 5.39      | 3.71      | 2.08      | 0.42      | 3.96      | 1.42      | 2.66      | 1.13       | 27.89 |
| 14  | 2.22      | 3.14      | 2.86      | 1.10      | 2.36      | 0.04      | 3.43      | 1.97      | 1.58       | 22.11 |
| 15  | 2.95      | 4.72      | 2.79      | 1.50      | 1.04      | 2.78      | 2.10      | 2.49      | 1.09       | 22.52 |
| 16  | 2.88      | 4.68      | 2.81      | 1.49      | 1.09      | 2.75      | 2.14      | 2.48      | 1.08       | 22.41 |
| 17  | 2.93      | 4.70      | 2.85      | 1.49      | 1.10      | 2.78      | 2.14      | 2.48      | 1.06       | 22.52 |
| 18  | 2.94      | 4.69      | 2.87      | 1.50      | 1.01      | 2.87      | 2.06      | 2.50      | 1.06       | 22.80 |
| 19  | 2.97      | 4.71      | 2.89      | 1.51      | 0.95      | 2.92      | 2.02      | 2.50      | 1.07       | 22.96 |
| 20  | 2.97      | 4.70      | 2.90      | 1.50      | 0.93      | 2.95      | 2.00      | 2.51      | 1.07       | 23.02 |

$R_{i, i+1}$ : resolution between the adjacent peaks  $i$  and  $i+1$ ;  $T_L$ : analysis time of the last interested peak.

表S4 星点设计实验的方差分析

Table S4 Analysis of variance of CCD

| Factor         | Degree of freedom | Sum of squared | Mean square | <i>F</i> | <i>P</i> |
|----------------|-------------------|----------------|-------------|----------|----------|
| Regression     | 9                 | 496.079        | 55.12       | 103.21   | <0.001   |
| Linear         | 3                 | 96.214         | 32.071      | 60.05    | <0.001   |
| $X_1$          | 1                 | 32.274         | 32.274      | 60.43    | <0.001   |
| $X_2$          | 1                 | 13.909         | 13.909      | 26.04    | <0.001   |
| $X_3$          | 1                 | 50.031         | 50.031      | 93.68    | <0.001   |
| Square         | 3                 | 211.329        | 70.443      | 131.9    | <0.001   |
| $X_1^2$        | 1                 | 146.917        | 146.917     | 275.1    | <0.001   |
| $X_2^2$        | 1                 | 84.4           | 84.4        | 158.04   | <0.001   |
| $X_3^2$        | 1                 | 4.53           | 4.53        | 8.48     | 0.015    |
| Interaction    | 3                 | 188.537        | 62.846      | 117.68   | <0.001   |
| $X_1X_2$       | 1                 | 3.668          | 3.668       | 6.87     | 0.026    |
| $X_1X_3$       | 1                 | 2.932          | 2.932       | 5.49     | 0.041    |
| $X_2X_3$       | 1                 | 181.937        | 181.937     | 340.67   | <0.001   |
| Residual error | 10                | 5.341          | 0.543       | /        | /        |
| Lack of fit    | 5                 | 3.47           | 0.694       | 1.86     | 0.257    |
| Pure error     | 5                 | 1.87           | 0.371       | /        | /        |
| Sum            | 19                | 501.42         | /           | /        | /        |

$X_1$ ,  $X_2$ ,  $X_3$  are the same as in Table S1. *P*: chi-square test; /: unavailable.