

**Supplementary data****Table S1.** Analytical performances of HPLC analysis of 25 µg/mL charantin

| Peak no. | Name                            | RT (min) | Area    | R <sub>s</sub> | TF  | k'    | N      |
|----------|---------------------------------|----------|---------|----------------|-----|-------|--------|
| 1        | Sterol derivative               | 14.5     | 95,286  | -              | 1.0 | 0     | 16,992 |
| 2        | 5, 25-Stigmastadienol glucoside | 15.5     | 227,880 | 2.0            | 0.9 | 0.065 | 16,401 |
| 3        | <i>β</i> -Sitosterol glucoside  | 22.4     | 37,287  | 12.5           | 1.0 | 0.544 | 19,278 |

**Table S2.** Validation data

| Parameter                        | Results                            |          |
|----------------------------------|------------------------------------|----------|
| Calibration curve                | Range (µg/mL)                      | <i>r</i> |
| • Sterol derivative              | 1-50                               | 0.9979   |
| • 5,25-Stigmastadienol glucoside | 1-50                               | 0.9990   |
| • $\beta$ -Sitosterol glucoside  | 1-50                               | 0.9993   |
| • Charantin                      | 1-50                               | 0.9994   |
| Precision                        | %RSD                               |          |
| • Repeatability                  |                                    |          |
| - Sterol derivative              | 0.9-2.7                            |          |
| - 5,25-Stigmastadienol glucoside | 1.1-3.1                            |          |
| - $\beta$ -Sitosterol glucoside  | 1.0-3.5                            |          |
| - Charantin                      | 0.8-3.4                            |          |
| • Reproducibility                |                                    |          |
| - Sterol derivative              | 1.2-3.7                            |          |
| - 5,25-Stigmastadienol glucoside | 3.0-3.9                            |          |
| - $\beta$ -Sitosterol glucoside  | 2.0-3.8                            |          |
| - Charantin                      | 1.1-3.7                            |          |
| Accuracy                         |                                    |          |
| • %Recovery                      | Mean recoveries $\pm$ SD           |          |
| - Sterol derivative              | 101.7 $\pm$ 2.4 to 106.1 $\pm$ 1.9 |          |
| - 5,25-Stigmastadienol glucoside | 96.9 $\pm$ 2.6 to 101.9 $\pm$ 2.1  |          |
| - $\beta$ -Sitosterol glucoside  | 97.7 $\pm$ 1.2 to 102.3 $\pm$ 3.0  |          |
| - Charantin                      | 98.9 $\pm$ 2.5 to 101.9 $\pm$ 3.2  |          |
| LOQs                             | µg/mL (%RSD)                       |          |
| • Sterol derivative              | 1.0 (2.7)                          |          |
| • 5,25-Stigmastadienol glucoside | 1.0 (2.8)                          |          |
| • $\beta$ -Sitosterol glucoside  | 0.5 (3.1)                          |          |
| LODs                             | µg/mL                              |          |
| • Sterol derivative              | 0.34                               |          |
| • 5,25-Stigmastadienol glucoside | 0.34                               |          |
| • $\beta$ -Sitosterol glucoside  | 0.17                               |          |

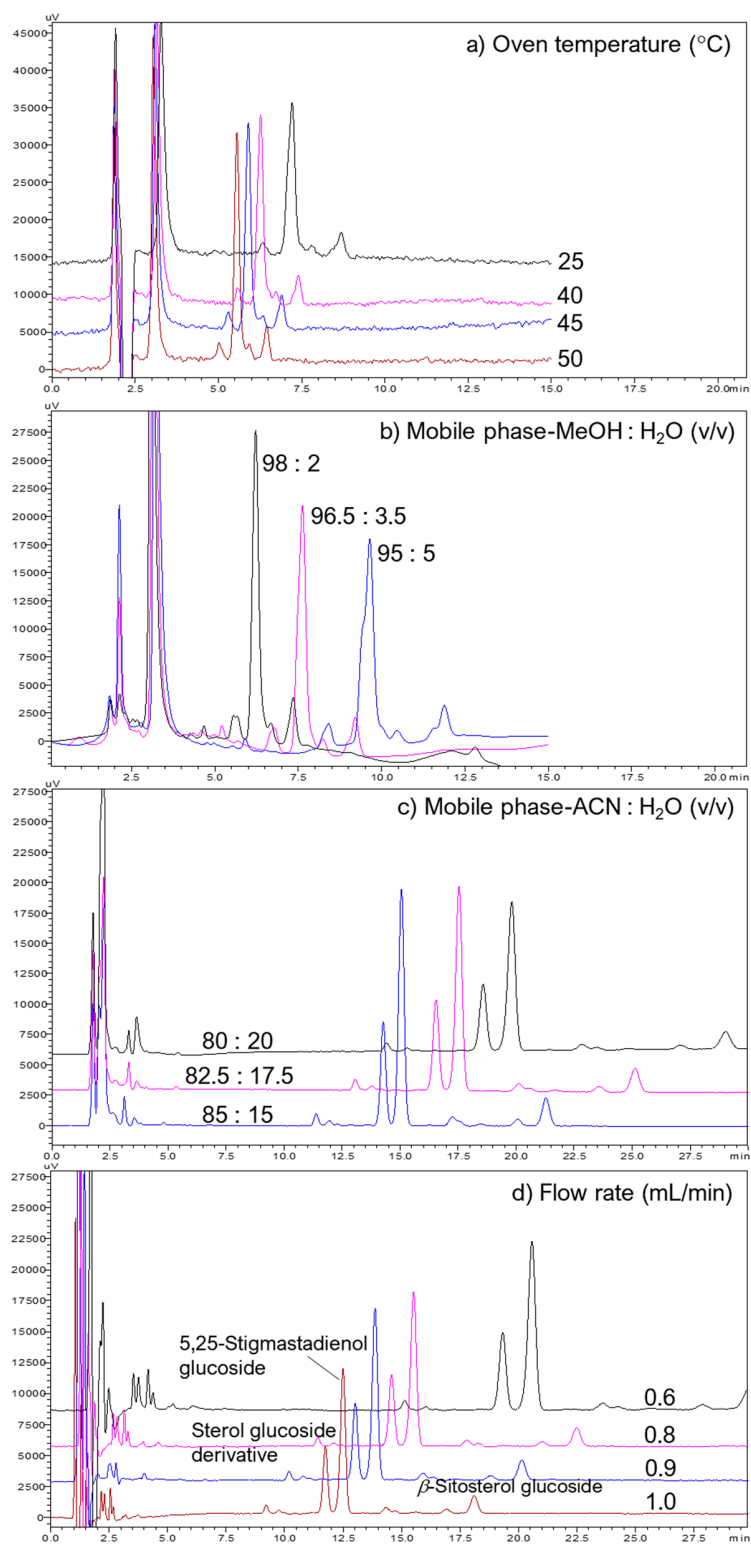
**Table S3.** Fit statistics of the model for the measured responses

| Responses                  | F-value | <i>p</i> -value | R <sup>2</sup> | Adjusted R <sup>2</sup> | Predicted R <sup>2</sup> | Adeq. Precision |
|----------------------------|---------|-----------------|----------------|-------------------------|--------------------------|-----------------|
| Imprinting factor (IF)     | 48.99   | < 0.0001        | 0.9169         | 0.8982                  | 0.8676                   | 26.2467         |
| Extraction efficiency (EE) | 103.27  | < 0.0001        | 0.9588         | 0.9495                  | 0.9381                   | 38.0388         |

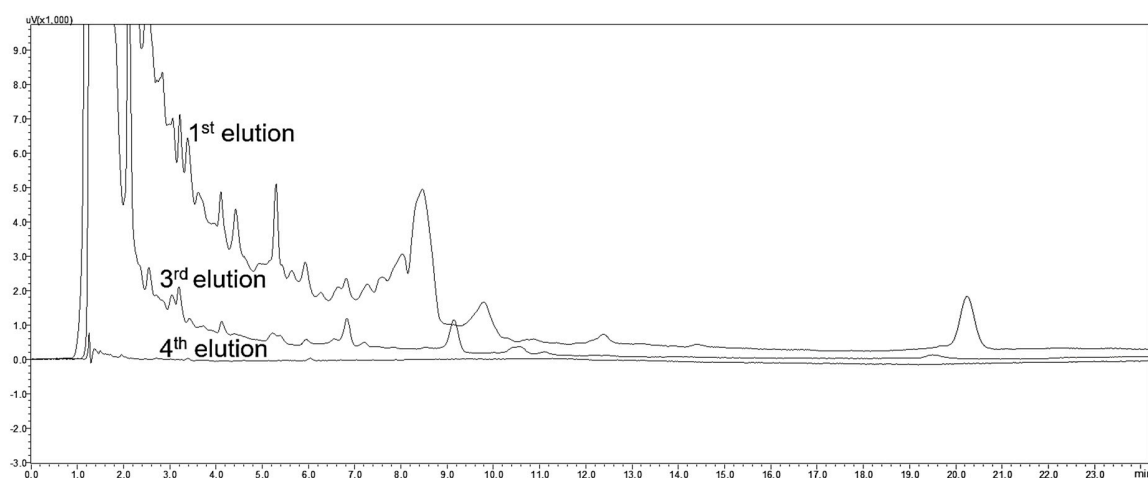
**Table S4.** Charantin content extracted from *M. charantia* powder by liquid-liquid extraction (LLE) and Fe<sub>3</sub>O<sub>4</sub>@MIPs

| Charantin constituent          | Content <sup>a</sup> (mg/100 g dry weight) |                                      |                 |             |                                      |                 |
|--------------------------------|--|--------------------------------------|-----------------|-------------|--------------------------------------|-----------------|
|                                | P1   |                                      | <i>p</i> -value | P2          |                                      | <i>p</i> -value |
|                                | LLE  | Fe <sub>3</sub> O <sub>4</sub> @MIPs |                 | LLE         | Fe <sub>3</sub> O <sub>4</sub> @MIPs |                 |
| Sterol glucoside               | 53.0 ± 9.8                                 | 135.2 ± 7.1                          | 0.000           | 44.2 ± 2.4  | 112.4 ± 15.6                         | 0.002           |
| 5,25-Stigmastadienol glucoside | 51.3 ± 7.6                                 | 126.0 ± 5.8                          | 0.000           | 45.9 ± 2.5  | 109.1 ± 14.1                         | 0.002           |
| <i>β</i> -Sitosterol glucoside | 18.7 ± 3.3                                 | 38.5 ± 2.3                           | 0.001           | 123.4 ± 4.7 | 179.5 ± 14.9                         | 0.003           |

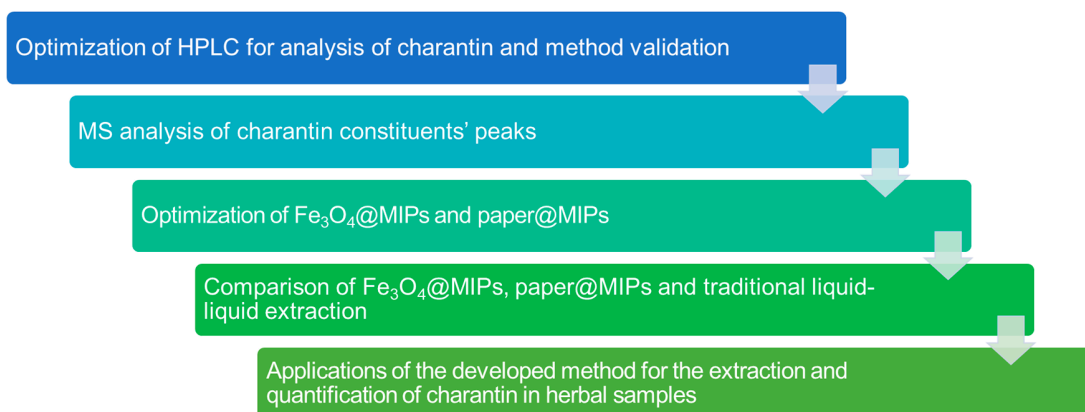
<sup>a</sup> Data are expressed as mean ± SD (n = 3).



**Figure S1.** Effects of (a) oven temperature, (b) methanol content in mobile phase, (c) acetonitrile content in mobile phase and (d) flow rate on the chromatographic separation of charantin.



**Figure S2.** HPLC analysis of eluates obtained from the washing step of MIPs for removal of the template and unreacted monomers.



**Figure S3.** Overall methodologies