

Supplementary Material

Semi-synthetic approach leading to 8-prenylnaringenin and 6-prenylnaringenin: Optimization of the microwave-assisted demethylation of xanthohumol using Design of Experiments

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Table S 1. Experimental plan 1 and maximum pressure.

| Block | Temperatur (°C) | LiCl (mg) | Time (min) | Maximum Pressure (bar) |
|-------|--------------------|--------------|---------------|---------------------------|
| 1 | 190 | 13.4 | 17.5 | 3 |
| 1 | 160 | 23.77 | 30 | 0 |
| 1 | 160 | 2.54 | 5 | 0 |
| 1 | 220 | 2.5 | 5 | 6 |
| 1 | 190 | 13 | 17.5 | 3 |
| 1 | 160 | 2.6 | 30 | 1 |
| 1 | 190 | 13.46 | 17.5 | 3 |
| 1 | 220 | 23.8 | 30 | 7 |
| 1 | 220 | 23.9 | 5 | 7 |
| 1 | 160 | 24 | 5 | 0 |
| 1 | 220 | 2.6 | 30 | 7 |
| 2 | 190 | 13.2 | 5 | 3 |
| 2 | 190 | 2.32 | 17.5 | 3 |
| 2 | 135 | 13.06 | 17.5 | 0 |
| 2 | 190 | 13.19 | 40 | 3 |
| 2 | 190 | 13.23 | 17.5 | 3 |
| 2 | 244 | 13.49 | 17.5 | 9 |
| 2 | 190 | 32.32 | 17.5 | 4 |
| 2 | 190 | 13.14 | 17.5 | 3 |
| 2 | 190 | 13.29 | 17.5 | 3 |

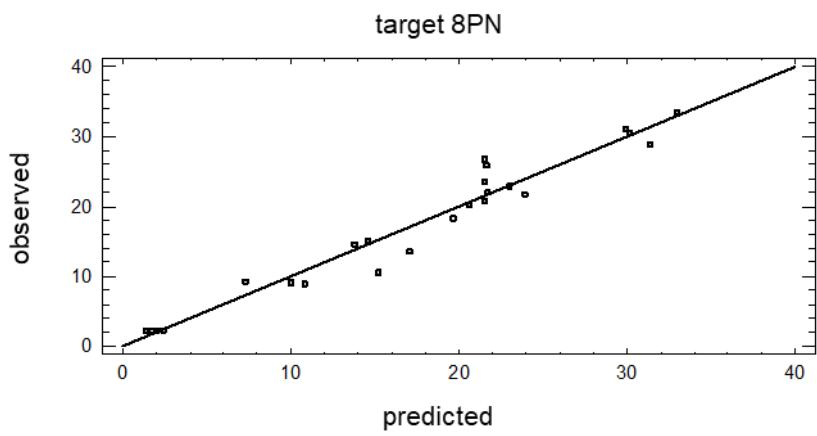


Figure S 1. Plot observed versus predicted values for the target '8PN'.

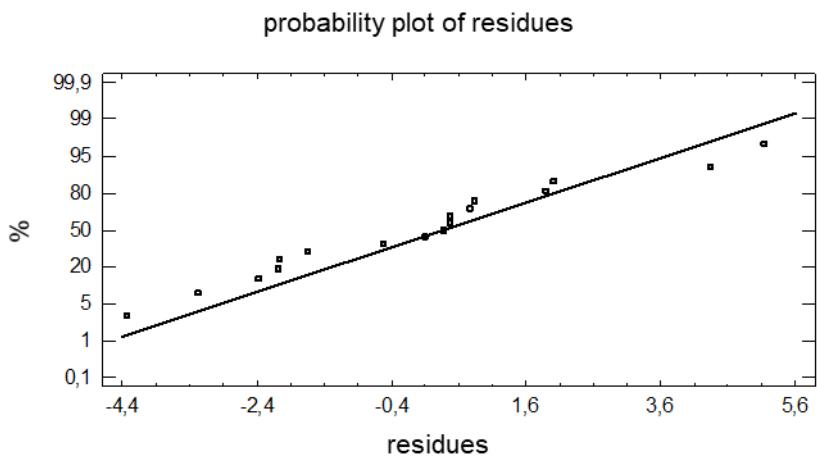


Figure S 2. Interaction plot of target '8PN'.

Table S 2. Experimental plan 2 and maximum pressure.

| Block | Temperatur (°C) | LiCl (mg) | Time (min) | Maximum Pressure (bar) |
|-------|--------------------|--------------|---------------|------------------------------|
| 1 | 205 | 36.81 | 1 | 4 |
| 1 | 190 | 47.89 | 1 | 3 |
| 1 | 205 | 36.79 | 5 | 4 |
| 1 | 205 | 37.18 | 5 | 4 |
| 1 | 205 | 37 | 5 | 6 |
| 1 | 220 | 47.55 | 9 | 6 |
| 1 | 180 | 37.13 | 5 | 2 |
| 1 | 190 | 26.98 | 1 | 3 |
| 1 | 190 | 47.65 | 9 | 3 |
| 1 | 205 | 36.63 | 11.7 | 5 |
| 1 | 205 | 37.45 | 5 | 4 |
| 1 | 220 | 47.83 | 1 | 6 |
| 1 | 205 | 37.3 | 5 | 5 |
| 1 | 220 | 26.25 | 1 | 8 |

| | | | | |
|---|-----|-------|------|---|
| 1 | 205 | 54.87 | 5 | 4 |
| 1 | 205 | 19.79 | 5 | 6 |
| 1 | 220 | 26.54 | 9 | 8 |
| 1 | 230 | 37.41 | 5 | 9 |
| 1 | 190 | 26.91 | 9 | 3 |
| 2 | 200 | 55.87 | 11.7 | 4 |
| 3 | 200 | 65.35 | 7.27 | 4 |

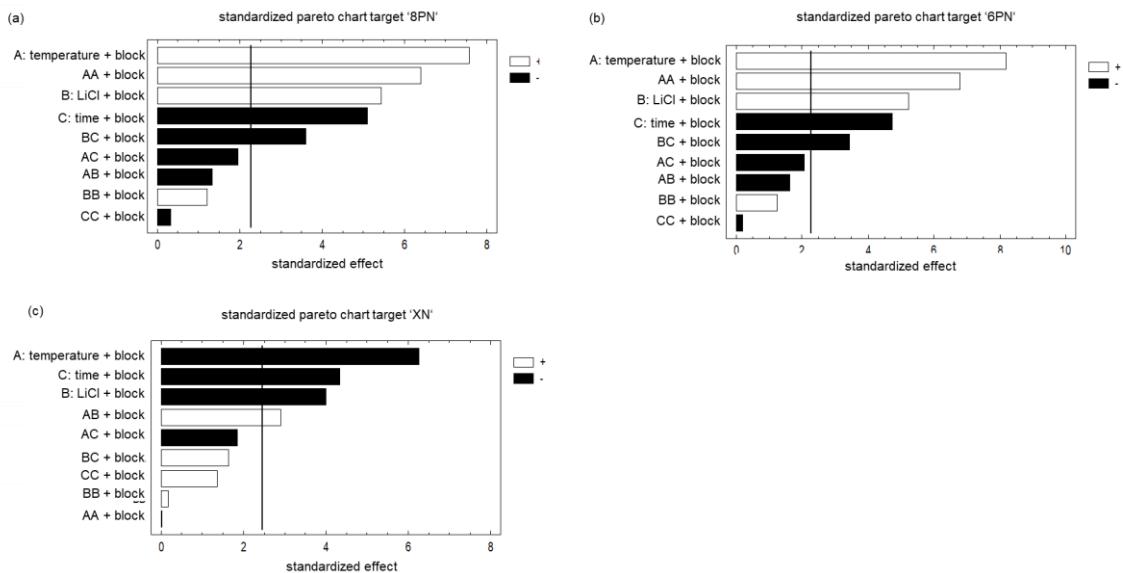


Figure S 3. Standardized pareto charts for targets '8PN', '6PN' and 'XN'.

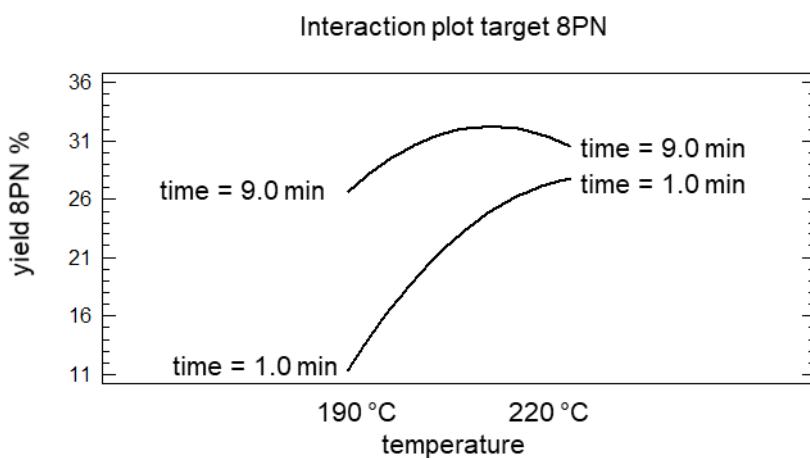


Figure S 4. Interaction plot of target '8PN'