

Supplementary Table 3. Goodness-of-fit indicators between experimental expressions and model simulations.

| Target gene     | Dataset                        | R <sup>2</sup>                      | RMSE                   |
|-----------------|--------------------------------|-------------------------------------|------------------------|
| <i>SIHY5</i>    | Training (Zhang et al. 2020)   | 0.8965                              | 0.1654                 |
| <i>SIMYB15</i>  | Training (Zhang et al. 2020)   | 0.8362(WT)/0.9175(mutant)/0.885(OE) | 0.23506/0.1301/0.36965 |
| <i>SICBF1</i>   | Validation (Zhang et al. 2004) | 0.8434/0.9859                       | 0.58285/0.1937         |
| <i>SICOR413</i> | Validation (Zhang et al. 2021) | 0.9283                              | 0.09034                |