

## An efficient biomimetic Fe-catalyzed epoxidation of olefins using hydrogen peroxide.

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### Supporting information

**Table 1.** Base effect of Fe-catalyzed epoxidation of *trans*-stilbene

5 mol% FeCl<sub>3</sub>·6H<sub>2</sub>O, 5 mol% H<sub>2</sub>pydic, 10 mol% Base  
3 equiv. H<sub>2</sub>O<sub>2</sub>, *t*-AmylOH, rt, 1 h addition

| Entry | Base                     | Conv. (%) <sup>a,b</sup> | Yield (%) <sup>b</sup> | Selec. (%) <sup>c</sup> | Entry     | Base                      | Conv. (%) <sup>a,b</sup> | Yield (%) <sup>b</sup> | Selec. (%) <sup>c</sup> |
|-------|--------------------------|--------------------------|------------------------|-------------------------|-----------|---------------------------|--------------------------|------------------------|-------------------------|
| 1     | -                        | 0                        | 0                      | 0 <sup>d,e</sup>        | 13        | 1-Methyl-imidazole        | 78                       | 72                     | 92 <sup>f</sup>         |
| 2     | NaOAc                    | 50                       | 43                     | 86 <sup>e</sup>         | 14        | 2-Methyl-imidazole        | 12                       | 11                     | 92 <sup>f</sup>         |
| 3     | KOH                      | 33                       | 30                     | 91 <sup>e</sup>         | 15        | <b>4-Methyl-imidazole</b> | <b>100</b>               | <b>97</b>              | <b>97<sup>f</sup></b>   |
| 4     | NaHCO <sub>3</sub>       | 67                       | 63                     | 94 <sup>e</sup>         | 16        | 1-Butyl-imidazole         | 99                       | 95                     | 96 <sup>f</sup>         |
| 5     | KO <sup>t</sup> Bu       | 80                       | 42                     | 52 <sup>e</sup>         | 17        | 1-Benzyl-imidazole        | 97                       | 90                     | 93 <sup>f</sup>         |
| 6     | Cyclohexyl amine         | 61                       | 59                     | 97                      | 18        | 1-Phenyl-imidazole        | 95                       | 85                     | 89 <sup>f</sup>         |
| 7     | <b>Bn-NH<sub>2</sub></b> | <b>100</b>               | <b>97</b>              | <b>97</b>               | 19        | Pyridine                  | 56                       | 50                     | 89 <sup>e</sup>         |
| 8     | Et <sub>3</sub> N        | 86                       | 74                     | 86                      | <b>20</b> | <b>Pyrrolidine</b>        | <b>100</b>               | <b>97</b>              | <b>97</b>               |
| 9     | DMAP                     | 19                       | 16                     | 84 <sup>e</sup>         | 21        | ( <i>S</i> )-Prolinol     | 89                       | 89                     | >99                     |
| 10    | DABCO                    | 40                       | 33                     | 82 <sup>e</sup>         | 22        | -                         | 7                        | 4                      | 57 <sup>g</sup>         |
| 11    | DBU                      | 41                       | 33                     | 80 <sup>e</sup>         | 23        | Pyrrolidine               | 0                        | 0                      | 0 <sup>h</sup>          |
| 12    | Imidazole                | 91                       | 90                     | 99                      | 24        | Pyrrolidine               | 0                        | 0                      | 0 <sup>g</sup>          |

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a) Reaction conditions: In a 25 mL Schlenk tube,  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$  (0.025 mmol),  $\text{H}_2\text{pydic}$  (0.025 mmol), *tert*-amyl alcohol (9 mL), base (0.05 mmol), *trans*-stilbene (0.5 mmol) and dodecane (GC internal standard, 100  $\mu\text{L}$ ) were added in sequence at rt in air. To this mixture, a solution of 30% hydrogen peroxide (170  $\mu\text{L}$ , 1.5 mmol) in *tert*-amyl alcohol (830  $\mu\text{L}$ ) was added over a period of 1 h at rt by a syringe pump. b) Conversion and yield were determined by GC analysis. c) Selectivity refers to the ratio of yield to conversion in percentage. d)  $\text{Na}_2\text{pydic}$  was used instead of  $\text{H}_2\text{pydic}$ . e)  $\text{H}_2\text{O}_2$  solution was added over a period of 12 h at rt by a syringe pump. f) 2 equiv. of  $\text{H}_2\text{O}_2$  was used. g)  $\text{H}_2\text{pydic}$  was not used. h)  $\text{FeCl}_3 \cdot 6\text{H}_2\text{O}$  was not used.