Supplementary Information

The generation of the oxidant agent of a mononuclear nonheme Fe(II) biomimetic complex by oxidative decarboxylation. A DFT investigation

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Table S1. Calculated spin contamination for all investigated complexes under all three spin states co spin states examined.

|        | 3     | 5     | 7     |
|--------|-------|-------|-------|
| a      | 2.0442| 6.0127| 12.0233|
| adduct | 3.5769| 6.6643| 12.0201|
| TS1    | 2.0210| 6.6945| 12.0188|
| hydroperoxo | 2.0294 | 6.1325 | 12.0182 |
| TS2    | 2.0361| 6.1380| -     |
| Prod   | 2.0334| 6.0156| 12.0297|
Figure S1 Crystal structure of hydrotris(3,5-diphenylpyrazole-1-yl)borate) Fe(II)-mandelate and its computational model (a) used in this study.
Figure S2 The two possible forms of the product of the oxidative decarboxylation process in quintet species.