Electronic Supplementary Material (ESI) for RSC Advances.

SUPPLEMENTARY MATERIAL

Figure S1: Transmission spectrum of the solid extracted from RhB oxidation reactions in the presence of m-CPBA and homogeneous (*S*,*S*)-Jacobsen P450-bioinspired catalyst (infrared region, 1% KBr tablet).

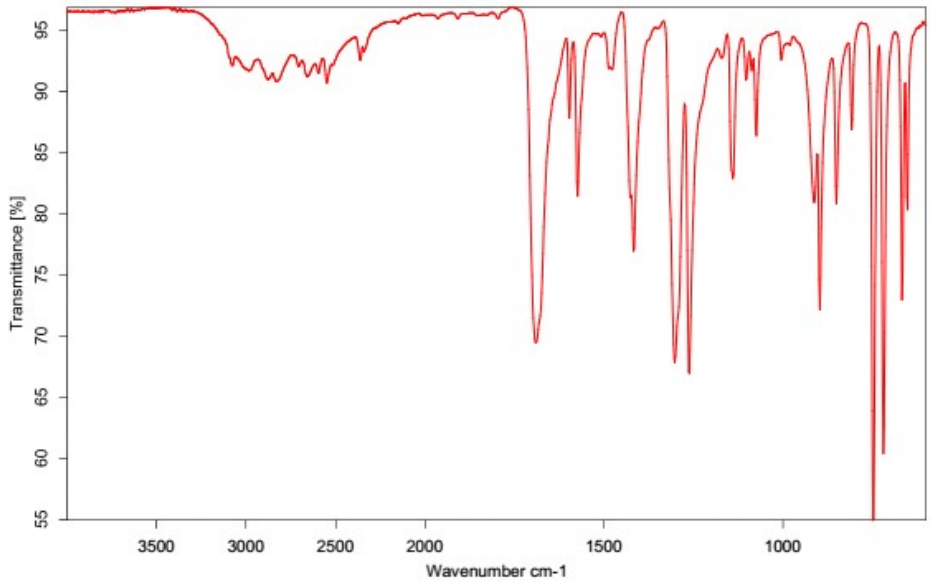
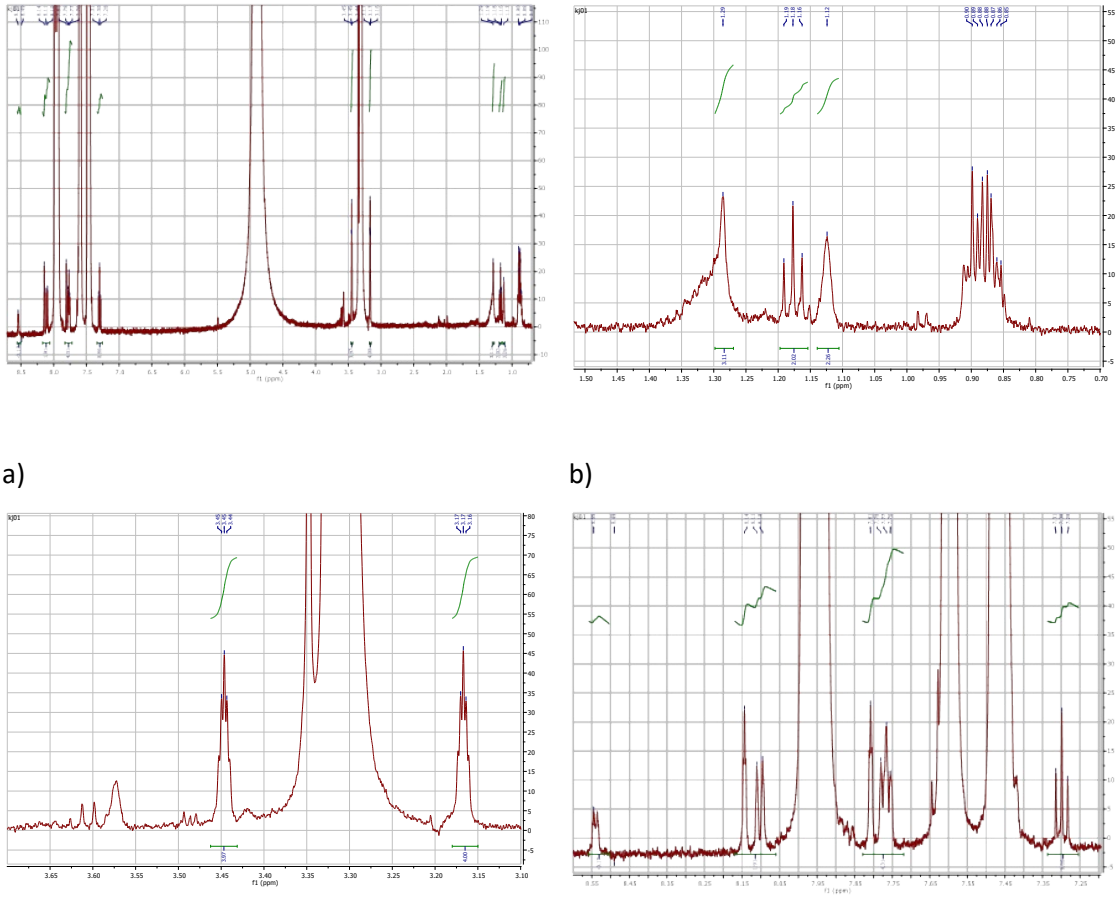


Figure S2: ^{1}H RMN spectrum of the possible oxidation products obtained by RhB oxidation reactions in the presence of *m*-CPBA and homogeneous (*S*,*S*)-Jacobsen P450-bioinspired catalyst. a) Full spectrum; b) expansion in the low field region; c) expansion of the middle field region; d) expansion of the aromatic hydrogen region.



a) b)

c) d)

It is noteworthy that a single NMR spectrum is not able to provide all the characterization evidence for these products. Because of this, we state that these are suggestions and not elucidations. Confirmation of products will be further supported with mass spectrometry in the future work. In addition, it is merit remembering that in a volume of 3 mL of reaction, the amount of substrate used was exceedingly small (1.25×10^{-4} mol) and consequently, the concentration of each product formed was much lower and thus, the signals recorded in the ^{1}H NMR analysis for this compound were exceptionally low.

A peculiar characteristic of Rhodamine B[1] is the presence of characteristic signs of the ethyl group (CH_3CH_2-), which results in a signal with quartet multiplicity (corresponding to the methylene hydrogens -CH_2-) and a singlet multiplicity sign (corresponding to the hydrogens of the methyl group -CH_3). These characteristic signs were not observed in the 1H NMR spectrum presented (Figure S2a). However, when expanding the spectrum

(Figures S2bcd), it is possible to observe the minority presence of substances that could be reaction products.

When analyzing Figure S2a, it is observed - immediately - that there are only 7 aromatic hydrogens. Compared to the expected 10 hydrogens, there is a reduction of 3, suggesting possible aromatic hydroxylations. Specifically, analyzing the Figures S2bc, a number of 15 hydrogens is observed, however, with multiplicity (Figure S2c) not corresponding to the quartet; but to a quintet (poorly solved). There are two signs with the same multiplicity, at 3.17 ppm and at 3.45 ppm, suggesting the lack of molecular symmetry.

Noticing the Figure S2b, it is possible to verify the presence of “grease” (between 0.85-0.90 ppm) and the following signals, totalling a quantity of 7 hydrogens. However, in these signals, there is no adequate and compatible resolution with the expected triplet. There are also 3 distinct signals, at 1.12 ppm (2H), 1.16-1.19 (3H) and 1.29 (2H), the latter being without adequate spectral resolution. Thus, it is possible to suggest a possible mix of products (Figure 8), including alkyl and aromatic hydroxylated products (singlet signals at 3.57, 3.60 and 3.61 ppm, respectively in Figure S2b).

1 SDBS AIST Database, https://sdbs.db.aist.go.jp/sdbs/cgi-bin/landingpage?sdbsno=15673 (accessed June 2021).