Supporting information for:

Vanadium-catalysed oxidative bromination using dilute mineral acids and hydrogen peroxide: an option for recycling waste acid streams / Gadi Rothenberg and James H. Clark.

As a basis for comparison, it is taken that bromination occurrs either using Br_2 (when present) or HOBr. The interconversions $HOBr + HBr \Leftrightarrow Br_2 + H_2O$, and $Br_2 + Br^- \Leftrightarrow Br_3^-$, are disregarded. The calculation of E-factors is based on the theoretical conversion of PhH to PhBr (assuming 100% yield).

Example (1). For the reaction $PhH + Br_2 \Rightarrow PhBr + HBr$, 80.9 g HBr (waste) for every 156.9 g PhBr (product) is produced, ergo E=80.9/156.9 = 0.51.

Example (2). When using $Br_2 + H_2O_2$, the reactions are:

$$PhH + Br_2 \longrightarrow PhBr + HBr \quad (6)$$

$$HBr + H_2O_2 \longrightarrow HOBr + H_2O \quad (7)$$

$$PhH + HOBr \longrightarrow PhBr + H_2O \quad (8)$$

$$2PhH + Br_2 + H_2O_2 \longrightarrow 2PhBr + 2H_2O \quad (9)$$

Resulting in 36 g H_2O (waste) for every 313.8 g PhBr (product), ergo E=36/313.8 = 0.11.