**SUPPORTING MATERIALS**

**Table 1S** The pKa results obtained by the linear programming method.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| pH | Ranitidine1 | Ranitidine2 | Nizatidine1 | Nizatidine2 | Doxylamine1 | Doxylamine2 | Carbinoxamine1 | Carbinoxamine2 |
| 3.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | **0** |
| 3.5 | 0 | 0 | 0 | 0 | 0 | 0 | **0** | 0 |
| 3.6 | 0 | 0 | 0 | 0 | 0 | 0 | **0** | 0 |
| 3.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 3.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.0 | 0 | 0 | 0 | 0 | **0** | **0** | 0 | 0 |
| 4.1 | 0 | 0 | 0 | 0 | **0** | **0** | 0 | 0 |
| 4.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 4.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.4 | 0 | 0 | 0 | 0 | 0 | **0.9341** | 0 | 0 |
| 5.5 | 0 | 0 | 0 | 0 | **1.4243** | **3.4595** | 0 | 0 |
| 5.6 | 0 | 0 | 0 | 0 | **1.5929** | 0 | 0 | 0 |
| 5.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 5.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.2 | 0 | 0 | 0 | 0 | 0 | 0 | **1.6652** | **1.5348** |
| 6.3 | 0 | 0 | 0 | 0 | 0 | 0 | **0.5291** | **0.6726** |
| 6.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 6.7 | 0 | 0 | **2.3665** | **2.6288** | 0 | 0 | 0 | 0 |
| 6.8 | 0 | 0 | **0.7283** | **0.6130** | 0 | 0 | 0 | 0 |
| 6.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 7.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.4 | **1.4792** | **1.8797** | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.5 | **1.0712** | **0.6892** | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 8.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.0 | 0 | 0 | 0 | 0 | 0 | 0 | **0.5746** | **0.1296** |
| 9.1 | 0 | 0 | 0 | 0 | 0 | 0 | **1.7453** | **2.0780** |
| 9.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.3 | 0 | 0 | 0 | 0 | **0.3530** | **0.7695** | 0 | 0 |
| 9.4 | 0 | 0 | 0 | 0 | **3.4751** | **3.3638** | 0 | 0 |
| 9.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 9.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.1 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.3 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.4 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.5 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.6 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.7 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 10.9 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 11.0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

**Figure 1S.** Reaction kinetics of 4 PPCPs oxidized by O3.



Fig. 1S

**Figure 2S.** Reaction kinetics of nizatidine oxidized by NaClO.



Fig. 2S

**Figure 3S.** Reaction kinetics of doxylamine oxidized by NaClO.





Fig. 3S

**Figure 4S.** Reaction kinetics of carbinoxamine oxidized by NaClO.





Fig. 4S

**Figure 5S.** Reaction kinetics of ranitidine oxidized by ClO2.





Fig. 5S

**Figure 6S.** Reaction kinetics of nizatidine oxidized by ClO2.





Fig. 6S

**Figure 7S.** Reaction kinetics of doxylamine oxidized by ClO2.



Fig. 7S

**Figure 8S.** Reaction kinetics of carbinoxamine oxidized by ClO2.





Fig. 8S

**Figure 9S.** Reaction kinetics of ranitidine oxidized by KMnO4.





Fig. 9S

**Figure 10S.** Reaction kinetics of nizatidine oxidized by KMnO4.





Fig. 10S

**Figure 11S.** Reaction kinetics of doxylamine oxidized by KMnO4.



Fig. 11S

**Figure 12S.** Reaction kinetics of carbinoxamine oxidized by KMnO4.



Fig. 12S