**Supplementary Material**

**Homogeneous continuous-flow nitration of *O*-methylisouronium sulfate and its optimization by kinetic modeling**

Jiapeng Guo a, Weike Su a, An Su a, b, \*

a Key Laboratory of Pharmaceutical Engineering of Zhejiang Province, Key Laboratory for Green Pharmaceutical Technologies and Related Equipment of Ministry of Education, Collaborative Innovation Center of Yangtze River Delta Region Green Pharmaceuticals, Zhejiang University of Technology, Hangzhou, 310014, P. R. China

b State Key Laboratory Breeding Base of Green Chemistry-Synthesis Technology, Key Laboratory of Green Chemistry-Synthesis Technology of Zhejiang Province, College of Chemical Engineering, Zhejiang University of Technology, Hangzhou, Zhejiang 310014, China

**\*Corresponding Author:**

Prof. An Su

<https://orcid.org/0000-0002-6544-3959>

Email: [ansu@zjut.edu.cn](mailto:ansu@zjut.edu.cn)

**Part 1. The effect of the external diffusion in batch reaction**



**Figure S1.** The effect of the external diffusion was eliminated in batch reaction. Reaction conditions: H2SO4 mass fractions = 98 %, reaction temperature T = 40 °C, residence time *t* = 2 min, Initial concentration of reactants = 1 mol/L, = 4.4 mol/L. The samples were quenched with excess ice water. The conversion were determined by high performance liquid chromatography (HPLC).

**Part 2. Effect of molar ratio**



**Figure S2.** Variation of NIO conversion with HNO3 molar ratio. The conversion was determined by high performance liquid chromatography (HPLC).

**Part 3. Determination of the reaction orders**



**Figure S3** (a). versus reaction time (*t*). (b). versus reaction time *t*. Determination of IO reaction order conditions: reaction temperature (T) = 0 °C; initial concentration of reactants in reaction mixture:  = 1 mol/L, = 15 mol/L; stirring speed = 1100 rpm. Determination of HNO3 reaction order conditions: reaction temperature (T) = 10 °C; initial concentration of reactants in reaction mixture: = 1 mol/L, =4.4 mol/L; stirring speed = 1100 rpm. The conversion was determined by high performance liquid chromatography (HPLC).

**Part** **4. Apparent reaction rate**



**Figure S4.** Variation of with *t* at different temperatures (30 ℃, 35 ℃, 40 ℃) and different H2SO4 mass fractions (88 %, 90 %, 92 %, 94%, 96 % 98 %).

**Part 5. Determination of function**



**Figure S5.** The results of polynomial fitting the data of function at 298K.[1]

**Part 6. Values of and under different temperatures and H2SO4 mass fraction**

**Table S1.** Values of and under different temperatures and H2SO4 mass fraction.

|  |  |  |  |
| --- | --- | --- | --- |
| **Mass fraction of H2SO4 (wt %)** | **Temperature (℃)** |  |  |
| 88 | 30 | 11.285 | -12.931 |
|  | 35 | 11.705 | -13.230 |
|  | 40 | 12.226 | -13.592 |
| 90 | 30 | 12.015 | -13.275 |
|  | 35 | 12.431 | -13.591 |
|  | 40 | 12.947 | -14.023 |
| 92 | 30 | 12.745 | -13.871 |
|  | 35 | 13.156 | -14.146 |
|  | 40 | 13.668 | -14.567 |
| 94 | 30 | 13.476 | -14.462 |
|  | 35 | 13.882 | -14.791 |
|  | 40 | 14.389 | -15.209 |
| 96 | 30 | 14.206 | -15.225 |
|  | 35 | 14.607 | -15.572 |
|  | 40 | 15.110 | -16.053 |
| 98 | 30 | 14.936 | -16.026 |
|  | 35 | 15.333 | -16.393 |
|  | 40 | 15.831 | -16.859 |

**References**

1. Marziano, N. C.; Tomasin, A.; Traverso, P. G. *Journal of the Chemical Society, Perkin Transactions 2* **1981**, (7), 1070-1075, 10.1039/P29810001070.