# Supplementary Information

## Degradation of benzotriazole and benzothiazole with the UV-activated peracetic acid process: performance, mechanism and transformation pathway

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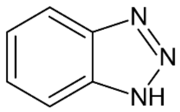
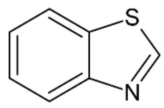
**Text S1.** Information on the chemicals used in this study.

BT (99%), BTH (96%), potassium phosphate monobasic ($KH_2PO_4$, 99%), potassium phosphate dibasic ($K_2HPO_4$, 98%), sodium chloride (NaCl, 99%), sodium nitrate ($NaNO_3$, 99%), *tert*-butanol (*t*-BuOH, 99%), sodium hydroxide (NaOH, 97%) and 5,5-dimethyl-1-pyrroline N-oxide (DMPO, 98%) were obtained from Sigma–Aldrich (St. Louis, MO, USA). Sodium thiosulfate ($Na_2S_2O_3$, 99%) was acquired from Alfa Aesar (Ward Hill, MA, USA). PAA (15%) was purchased from Ginyork (Taipei, Taiwan). Sodium bicarbonate (NaCl, 99.7%) and sulfuric acid were purchased from Fluka (Buchs, Switzerland). 2,2,6,6-Tetramethyl-4-piperidinol (TEMP, 98%) was obtained from Matrix Scientific (Columbia, SC, USA). Furfuryl alcohol (FFA, 98%) was acquired from Thermo Scientific (Waltham, MA, USA). HPLC-grade methanol was purchased from Duksan (Ansan, Korea), and LC–MS grade methanol was obtained from Macron Fine Chemicals (Center Valley, PA, USA). The Suwannee River fulvic acid standard (1S101F) was acquired from the International Humic Substance Society (IHSS; St. Paul, MN, USA). DPD total chlorine reagent powder pillows were obtained from HACH (Loveland, CO, USA). Milli-Q water (18.2 MΩ cm resistivity; Merck Millipore, MA, USA) was used in all solutions prepared in this study. All stock solutions were placed in amber glass containers and stored under dark conditions in a 4°C refrigerator until use.

**Table S1.** Physicochemical characteristics of BT and BTH.

| | BT | BTH |
|---|---|---|
| Chemical structure |  |  |
| Molecular formula | $C_6H_5N_3$ | $C_7H_5NS$ |
| Molecular weight (g/mol) | 119.12 | 135.19 |
| pka | 8.2[1] | 2.28[2] |
| log Kow | 1.23[3] | 1.99[4] |
| Water solubility (mg/L) | ~5957[5] | ~1684[5] |

He et al. (2002)[1]; Hernandez-Lopez et al. (2022)[2]; Hart et al. (2004)[3]; Reddy et al. (1997)[4]; Chemspider[5]

**Table S2.** Chromatographic conditions for the analyses of BT and BTH transformation products.

| | **BT transformation products** | **BTH transformation byproducts** |
|---|---|---|
| **Mode** | gradient | isocratic |
| **Total elution time** | 5.5 min | 3.5 min |
| **Mobile phases** | A: 0.1% formic acid in DI water<br>B: 0.1% formic acid in LCMS-grade methanol | A: 0.1% formic acid in DI water<br>B: 0.1% formic acid in LCMS-grade methanol |
| **Flow rate** | 0.4 mL/min | 0.4 mL/min |
| **Injection volume** | 20 μL | 20 μL |
| **Gradient conditions** | - 0 min: 95% (A): 5% (B)<br>- 0.5 min: 95% (A): 5% (B)<br>- 1 min: 5% (A): 95% (B)<br>- 3.5 min: 5% (A): 95% (B)<br>- 4 min: 95% (A): 5% (B)<br>- 5.5 min: 95% (A): 5% (B) | – |

**Table S3.** Mass spectrometric conditions for analyses of BT and BTH transformation products.

| | |
|---|---|
| **Mode** | ESI positive |
| **End plate offset voltage** | 500 V |
| **Capillary voltage** | 4500 V |
| **Nebulizer gas pressure** | 30.5 psi (2.1 bar) |
| **Dry gas flowrate** | 9 L/min |
| **Dry gas temperature** | 200 ℃ |
| **Mass scan range** | 50–500 m/z |

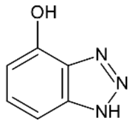
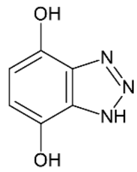
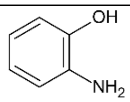
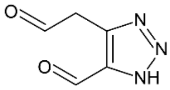
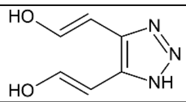
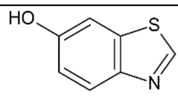
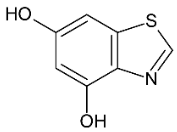
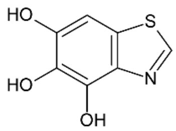
**Table S4.** UV/PAA degradation of various micropollutants and organic pollutants.

| Compound | Initial compound concentration | PAA dosage | Solution pH | Reaction time (min) | Removal efficiency | Reference |
|---|---|---|---|---|---|---|
| naproxen | 4 µM | 20 mg/L | 7 | 30 | 85% | (Chen et al., 2019)[6] |
| diclofenac | 1 µM | 50 µM | 7 | 15 | 80% | (Zhang et al., 2020)[7] |
| steroid estrogens (estrone, 17β-estradiol, estriol and 17α-ethinyl estradiol) | 50 µg/L | 30 mg/L | 6.01 | 30 | 80–100% | (Hu et al., 2022)[8] |
| ibuprofen | 1 µM | 1 mg/L | 7.1 | 30 | 90% | (Cai et al., 2017)[9] |
| bezafibrate | 1 µM | 1 mg/L | 7.1 | 120 | 90% | |
| clofibric acid | 1 µM | 1 mg/L | 7.1 | 10 | 90% | |
| tetracycline | 5 µM | 0.1 mM | 7 | 30 | 100% | (Meng et al., 2023)[10] |
| oxytetracycline | 5 µM | 0.1 mM | 7 | 45 | 100% | |
| chlortetracycline | 5 µM | 0.1 mM | 7 | 10 | 100% | |
| β-N-methylamino-L-alanine | 1 mg/L | 0.2 mM | 7 | 5 | 92.31% | (Zhou et al., 2022)[11] |
| haloanisoles (2-monochloroanisole, 2,4-dichloroanisole, 2,4,6-trichloroanisole and 2,4,6-tribromoanisole) | 50 µg/L | 10 mg/L | 5 | 60 | >92% | (Zhang et al., 2021)[12] |
| chloramphenicol | 25 mg/L | 50 mg/L | 7.6 | 120 | 100% | (Rizzo et al., 2018)[13] |
| benzotriazole | 0.08 mM | 10 mg/L | 7 | 25 | 100% | this work |
| benzothiazole | 0.08 mM | 10 mg/L | 7 | 40 | 91% | |

**Table S5.** Water quality of the WWTP wastewater sample.

| | pH | Alkalinity (mM $HCO_3^-$) | $NO_3^-$ (mM) | $Cl^-$ (mM) | Total organic carbon (mg/L) |
|---|---|---|---|---|---|
| WWTP wastewater | 7.02 | 1.71 | 0.97 | 0.63 | 9.5 |

**Table S6.** UHPLC–QTOF–MS information on the detected BT and BTH transformation products.

| **BT transformation products** | **Retention time (min)** | **Proposed structure** | **Proposed formula** | **Molecular mass (g/mol)** |
|---|---|---|---|---|
| BT-P1 | 2.9 |  | $C_6H_5N_3O$ | 135.12 |
| BT-P2 | 2.7 |  | $C_6H_5N_3O_2$ | 151.12 |
| BT-P3 | 1.3 |  | $C_6H_7NO$ | 109.13 |
| BT-P4 | 1.8 |  | $C_5H_5N_3O_2$ | 139.11 |
| BT-P5 | 1.1 |  | $C_6H_7N_3O_2$ | 153.14 |
| **BTH transformation products** | **Retention time (min)** | **Proposed structure** | **Proposed formula** | **Molecular mass (g/mol)** |
| BTH-P1 | 1.5 |  | $C_7H_5NOS$ | 151.19 |
| BTH-P2 | 0.9 |  | $C_7H_5NO_2S$ | 167.19 |
| BTH-P3 | 1.0 |  | $C_7H_5NO_3S$ | 183.18 |

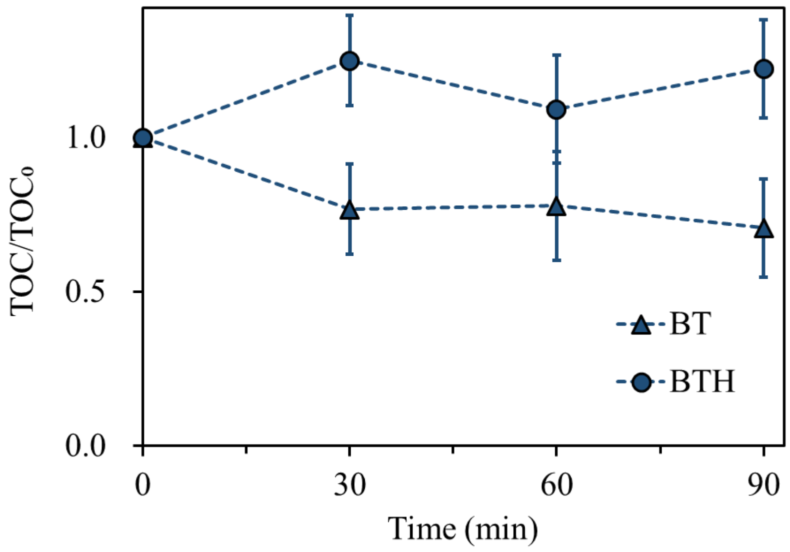



**Figure S1.** TOC mineralization of BT and BTH during the UV/PAA process ($[BT]_0$ or $[BTH]_0$ = 0.08 mM, $[PAA]_0$ = 10 mg/L and pH = 7.0).

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