

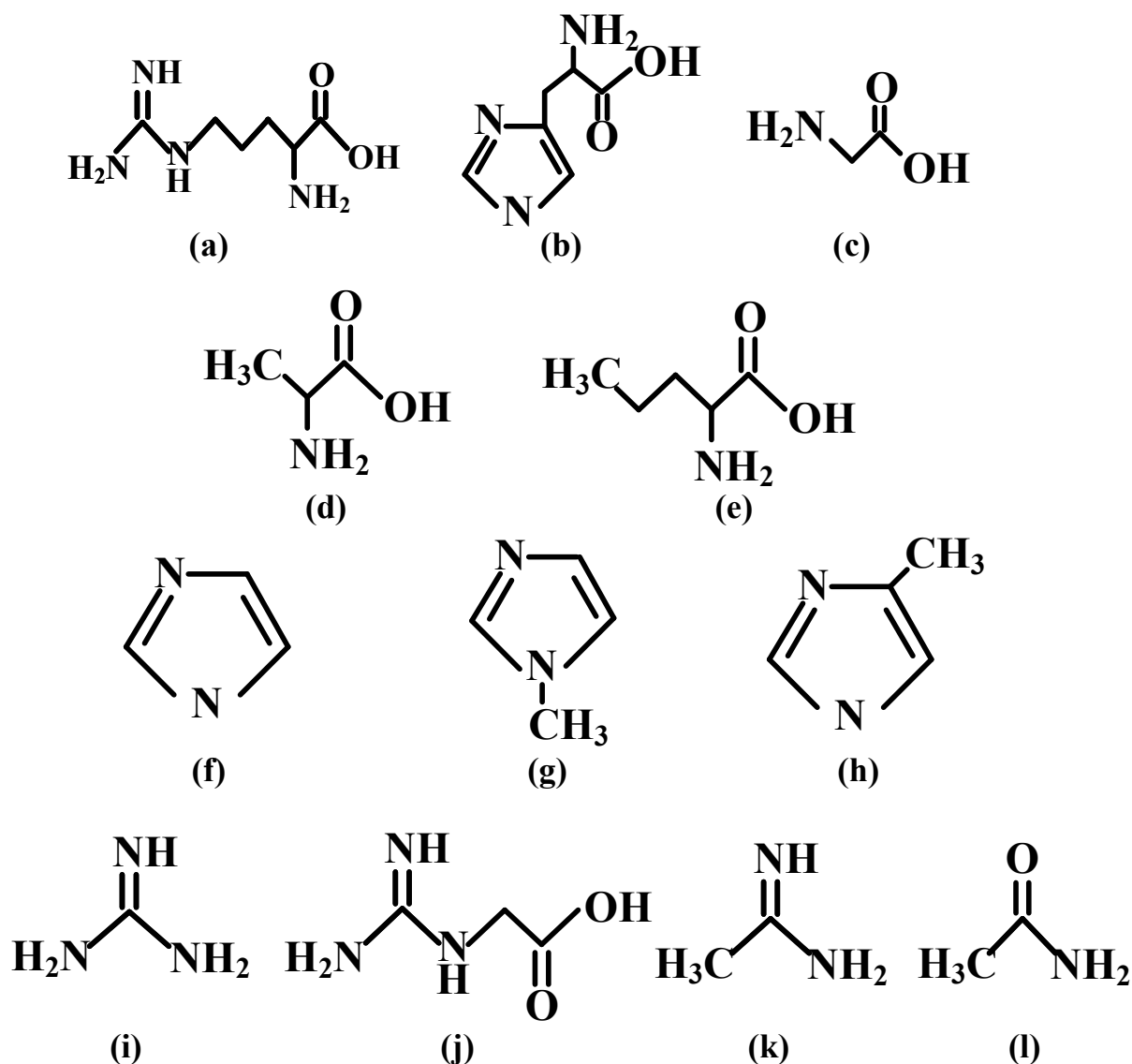
# **UV-Induced Effects on Chloramine and Cyanogen Chloride Formation from Chlorination of Amino Acids**

Shih Chi Weng<sup>1</sup> and Ernest R. Blatchley III<sup>1, 2\*</sup>

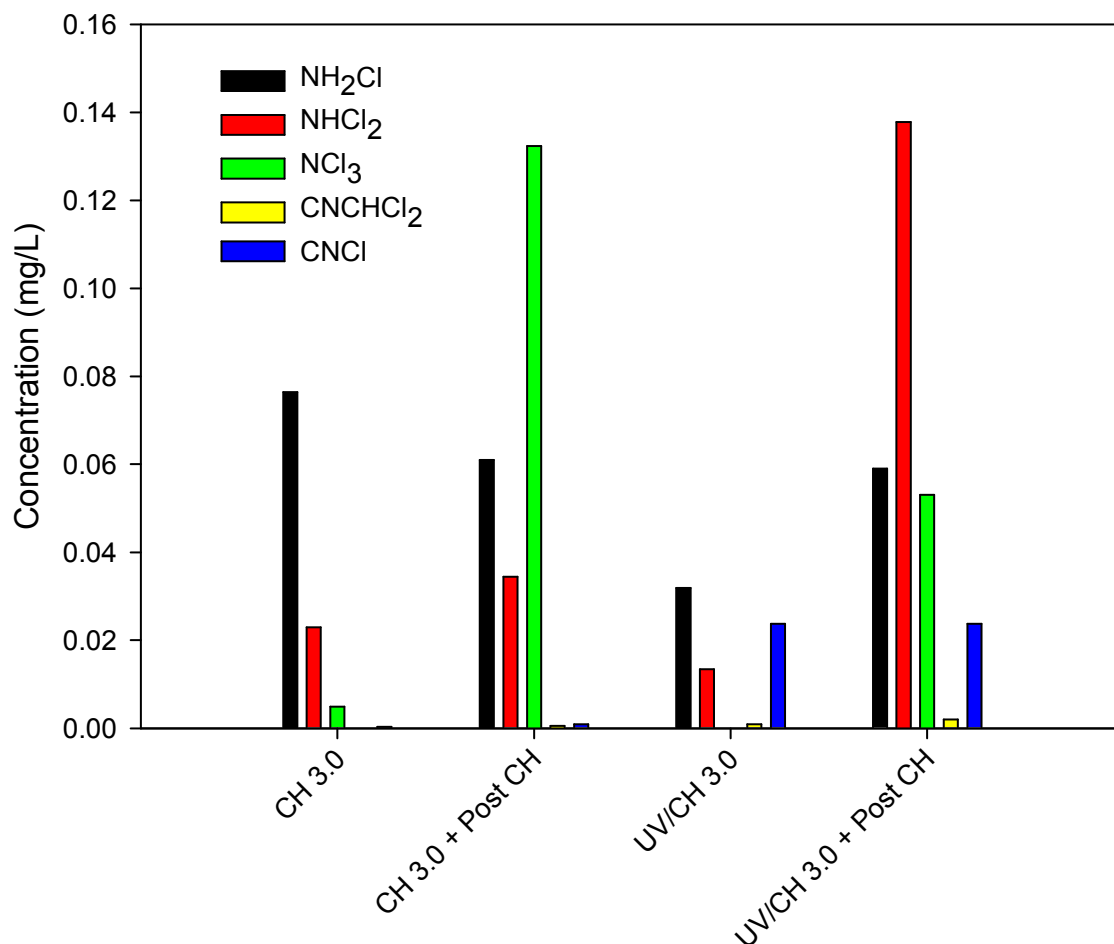
<sup>1</sup> School of Civil Engineering, Purdue University, IN 47906 USA

<sup>2</sup> Division of Environmental and Ecological Engineering, Purdue University, IN 47906 USA

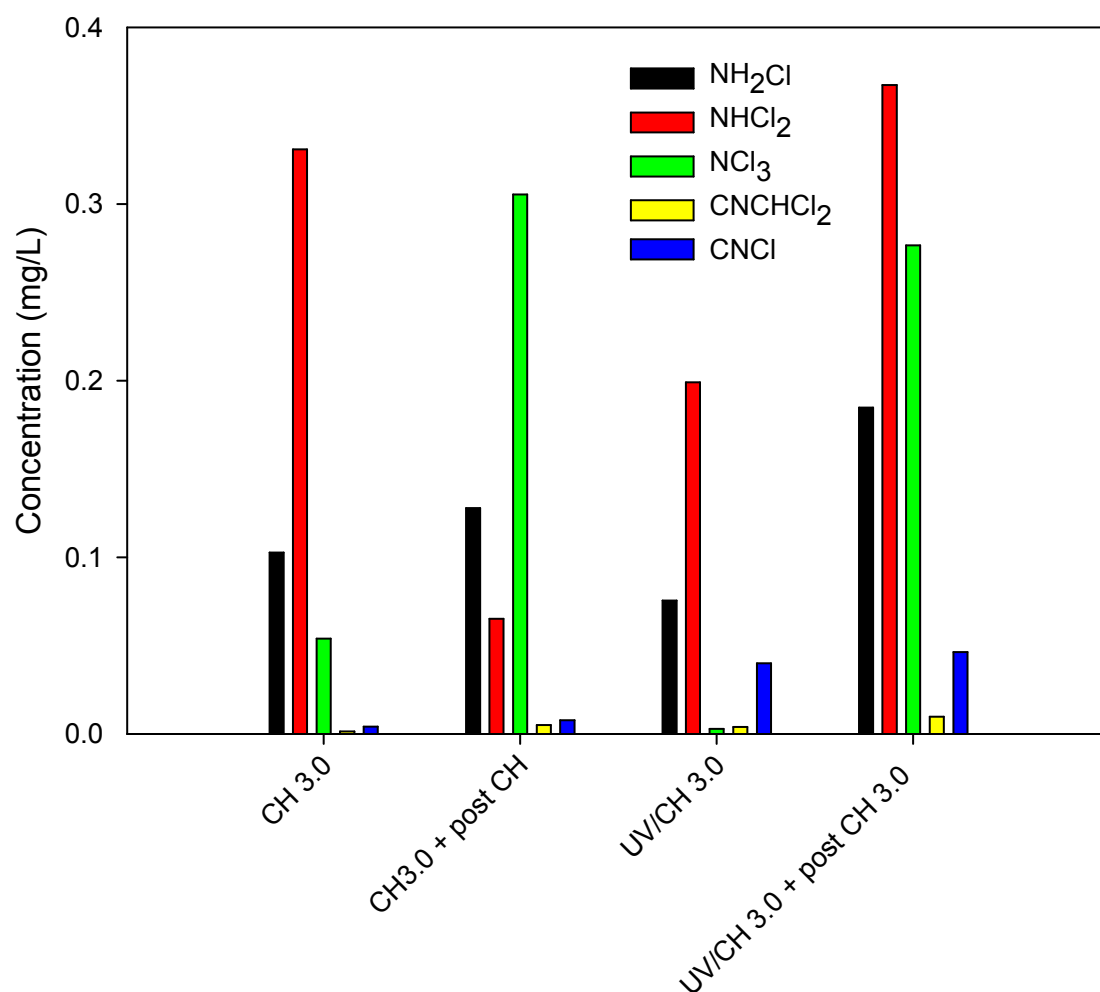
## **Supporting Information**



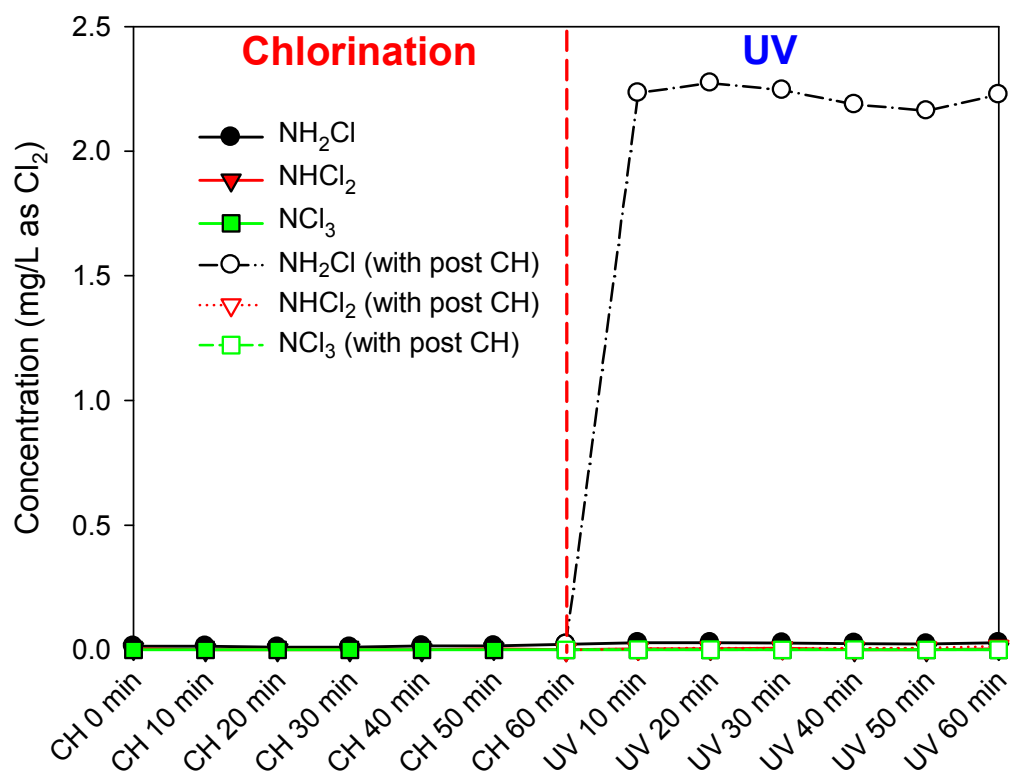
**Figure S1.** Structures of precursor compounds used in this study: (a) *L*-arginine (98%, Sigma-Aldrich), (b) *L*-histidine ( $\geq 99\%$ , Sigma-Aldrich), (c) glycine (99.4%, Sigma), (d) *L*-alanine (Sigma), (e) *L*-norvaline (sigma grade, Sigma-Aldrich), (f) imidazole ( $\geq 99\%$ , Sigma-Aldrich), (g) 1-methylimidazole (99%, Sigma-Aldrich), (h) 4-methylimidazole (98%, Aldrich), (i) guanidine ( $\geq 99\%$ , Sigma), (j) guanidineacetic acid (99%, Aldrich), (k) acetamidine (95%, Aldrich), and (l) acetamide (99%, Aldrich).



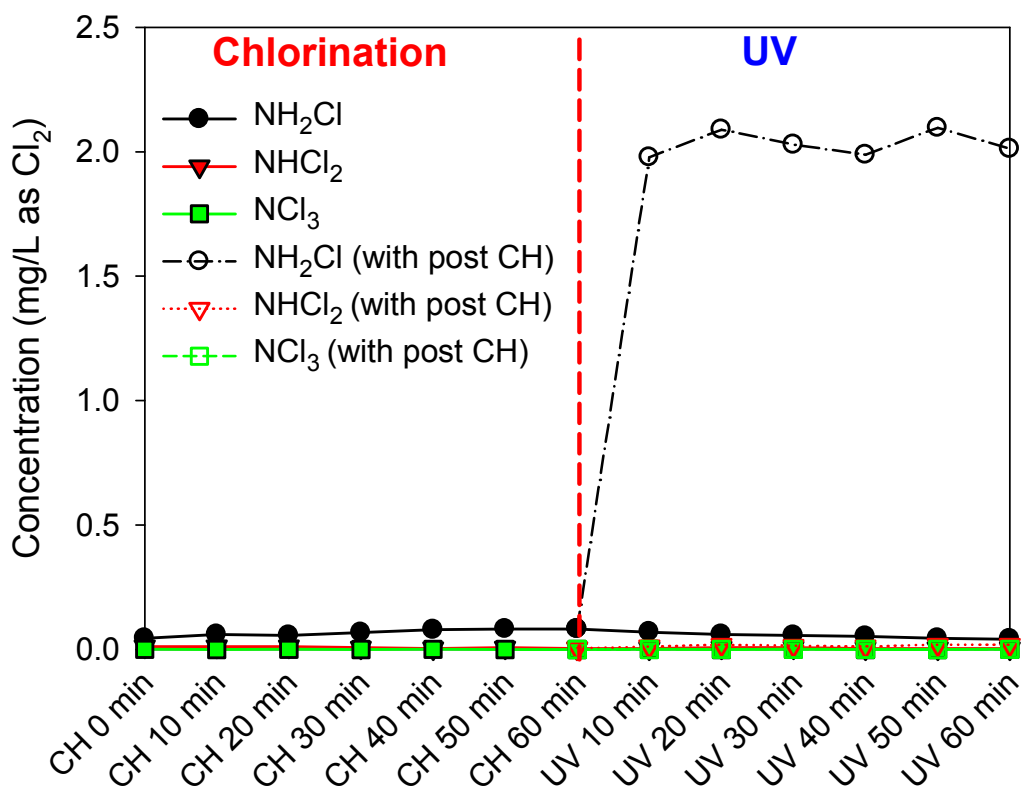
**Figure S2.** Formation of inorganic chloramines, CNCHCl<sub>2</sub>, and CNCl from *L*-arginine with sequential treatments of chlorination (CH), UV<sub>254</sub> irradiation (UV), and post-chlorination (post CH). The *L*-arginine solution was subjected to chlorination with Cl:P = 3.0 for 60 minutes (CH 3.0), chlorination with Cl:P = 3.0 for 60 minutes followed with post chlorination at 3 mg/L as Cl<sub>2</sub> (CH 3.0 + post CH), chlorination/UV<sub>254</sub> coexposure with Cl:P = 3.0 for 60 minutes (CH/UV 3.0), and coexposure of chlorine/UV with Cl:P = 3.0 for 60 minutes followed by post-chlorination at 3 mg/L as Cl<sub>2</sub> (CH/UV 3.0 + post CH).



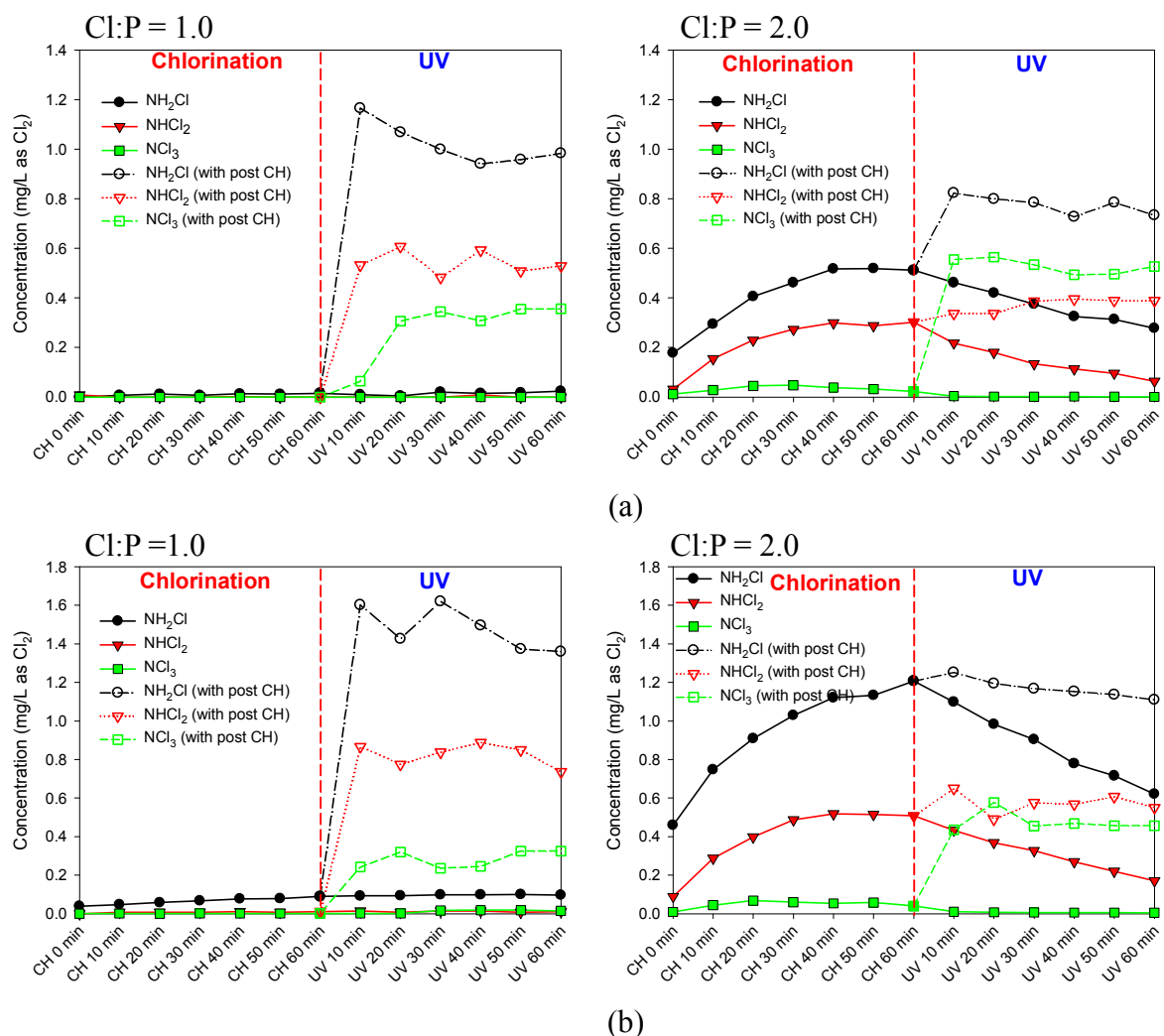
**Figure S3.** Formation of inorganic chloramines, CNCHCl<sub>2</sub>, and CNCl from *L*-histidine with sequential treatments of chlorination (CH), UV<sub>254</sub> irradiation (UV), and post-chlorination (post CH). The *L*-histidine solution was subjected to chlorination with Cl:P=3.0 for 60 minutes (CH 3.0), chlorination with Cl:P = 3.0 for 60 minutes followed with post chlorination at 3 mg/L as Cl<sub>2</sub> (CH 3.0 + post CH), chlorination/UV<sub>254</sub> coexposure with Cl:P =3.0 for 60 minutes (CH/UV 3.0), and coexposure of chlorine/UV with Cl:P = 3.0 for 60 minutes followed by post-chlorination at 3 mg/L as Cl<sub>2</sub> (CH/UV 3.0 + post CH).



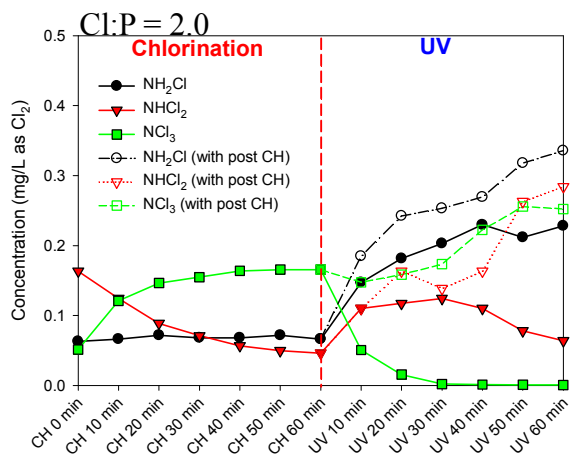
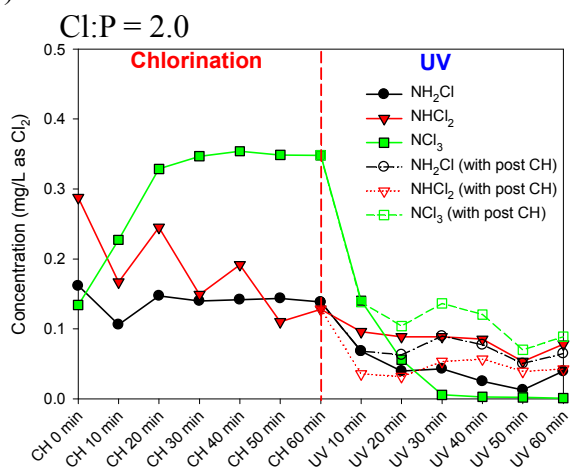
**Figure S4.** Time-course behavior of inorganic chloramines for samples of *L*-arginine (concentration =  $1.8 \times 10^{-4}$  M) subjected to chlorination for 60 minutes under Cl:P = 1.0, followed by UV<sub>254</sub> irradiation (solid lines and solid symbol) or UV<sub>254</sub> irradiation with post-chlorination (with post CH) at 3 mg/L as Cl<sub>2</sub> (dashed lines and open symbol). The experiment was intended to create a situation of chlorine:nitrogen molar ratio (Cl:N)  $\ll$  1 in post chlorination.



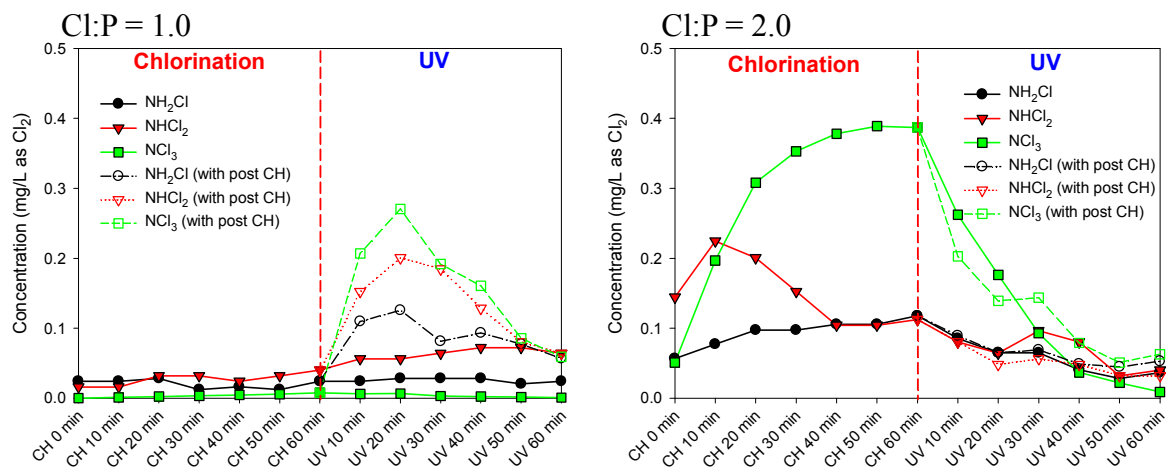
**Figure S5.** Time-course behavior of inorganic chloramines for samples of *L*-histidine (concentration =  $1.8 \times 10^{-4}$  M) subjected to chlorination for 60 minutes under Cl:P = 1.0, followed by UV<sub>254</sub> irradiation (solid lines and solid symbol) or UV<sub>254</sub> irradiation with post-chlorination (with post CH) at 3 mg/L as Cl<sub>2</sub> (dashed lines and open symbol). The experiment was intended to create a situation of chlorine:nitrogen molar ratio (Cl:N) << 1 in post chlorination.



**Figure S6.** Time-course behavior of inorganic chloramines for samples of (a) *L*-alanine, and (b) *L*-norvaline subjected to chlorination for 60 minutes (initial Cl:P = 1.0, and 2.0, left and right column, respectively) followed by  $\text{UV}_{254}$  irradiation (solid lines) or  $\text{UV}_{254}$  irradiation with post-chlorination (with post CH) at 3 mg/L as  $\text{Cl}_2$  (dashed lines).

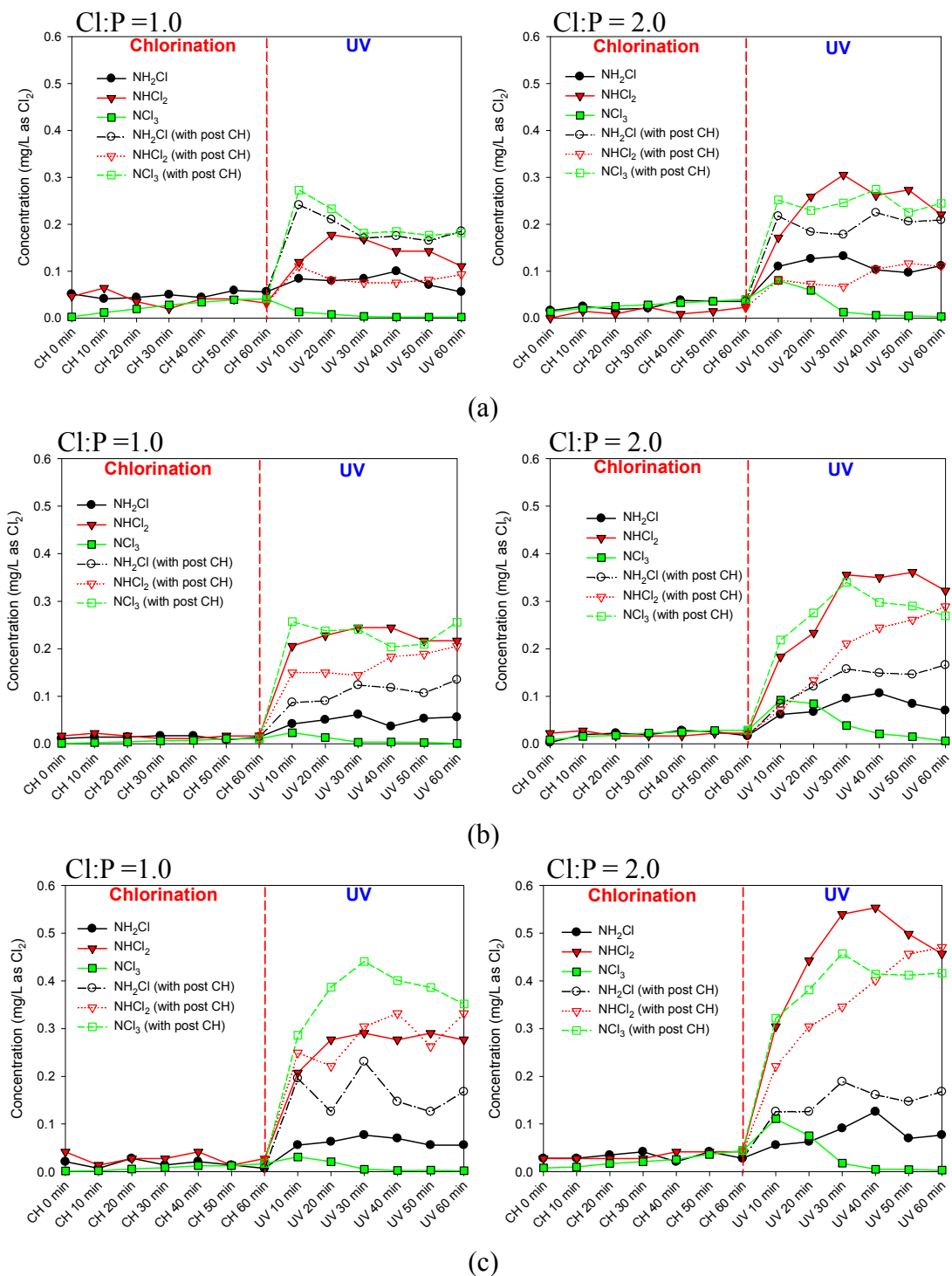




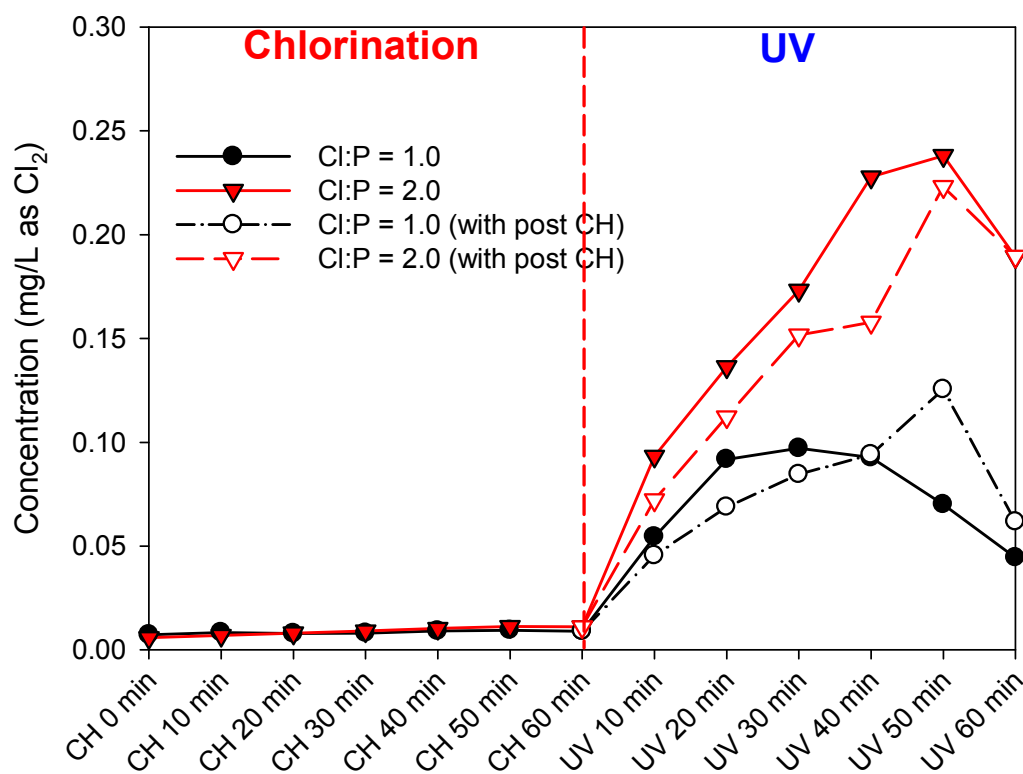


(d)

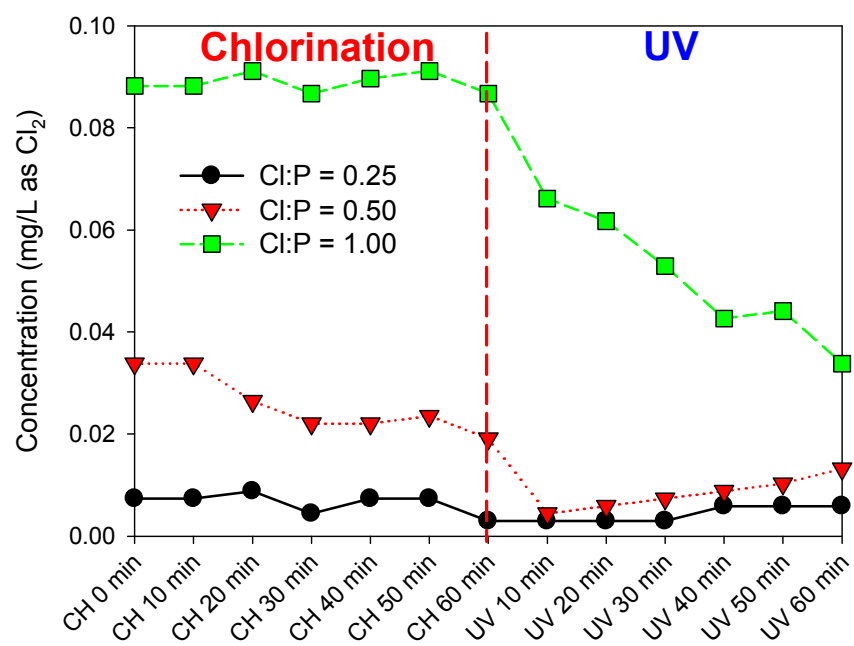
**Figure S7.** Time-course behavior of inorganic chloramines from guanidine compounds: (a) guanidine, (b) guanidineacetic acid, (c) acetamidine, and (d) acetamide subjected to chlorination for 60 minutes (initial Cl:P = 1.0 or 2.0; left and right column, respectively), followed by UV<sub>254</sub> irradiation (solid lines) or UV<sub>254</sub> irradiation with post-chlorination (with post CH) at 3 mg/L as Cl<sub>2</sub> (dashed lines).



**Figure S8.** Time-course behavior of inorganic chloramines for samples of imidazole compounds: (a) imidazole, (b) 1-methylimidazole, and (c) 4-methylimidazole subjected to chlorination for 60 minutes (initial Cl:P = 1.0 or 2.0; left and right column, respectively), followed by UV<sub>254</sub> irradiation (solid lines) or UV<sub>254</sub> irradiation with post-chlorination (with post CH) at 3 mg/L as Cl<sub>2</sub> (dashed lines).



**Figure S9.**  $\text{CH}_3\text{NCl}_2$  formation from chlorination/UV irradiation and post-chlorination (with post CH) experiments of 1-methylimidazole. Open symbols represent data from the post-chlorination experiment (dashed lines).



**Figure S10.**  $\text{NH}_2\text{Cl}$  formation from chlorination/ $\text{UV}_{254}$  irradiation experiments of glycine under  $\text{Cl:P} = 0.25$ ,  $0.5$ , and  $1.0$ .