

Appendix A. Supplementary data

Body fluid analog chlorination: Application to the determination of disinfection byproduct formation kinetics in swimming pool water

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Supporting information S1 – List of the chlorination experiments

Table S 1 List of the chlorination experiments

Compound or solution	Initial chlorine dose (mg/L as Cl ₂)	Total reaction time (h)	Parameters measured	Reference of the experiment
BFA mix	90	700	Free chlorine, TCM	BFA90
BFA mix	90	1920	TCM	BFA90L
BFA mix	90	10	TCM, DCAN	BFA90S
BFA mix	65	160	Free chlorine, TCM	BFA65
Urea	90	18	Free chlorine	U90
Urea	710	1	Free chlorine	U_DL_710 (De Laat et al., 2011)
Citric acid	10	30	TCM	CA10
Citric acid	30	160	Free chlorine, TCM	CA30
Citric acid	65	350	TCM	CA65
Citric acid	90	10	TCM	CA90S
Citric acid	90	270	TCM	CA90

Citric acid	90	1920	TCM	CA90L
Citric acid	20	120	TCM	CA_B_20 (Blatchley et al., 2003)
Creatinine	30	150	Free chlorine	C30
Creatinine	90	270	Free chlorine, TCM	C90
Creatinine	8,7	96	Free chlorine	C_B_10 (Li and Blatchley, 2007)
L-Histidine	5	170	Free chlorine, TCM, DCAN	H5
L-Histidine	10	27	TCM, DCAN	H10
L-Histidine	30	170	Free chlorine, TCM	H30
L-Histidine	30	20	DCAN	H30S
L-Histidine	60	10	DCAN	H60
L-Histidine	90	270	Free chlorine, TCM	H90
L-Histidine	90	10	DCAN	H90S
Uric acid	5	10	Free chlorine	UA5
Uric acid	30	170	Free chlorine	UA30
Uric acid	90	270	Free chlorine, TCM	UA90
Uric acid	17	72	Free chlorine	UA_L_20 (Lian et al., 2014)
Uric acid	28	72	Free chlorine	UA_L_30 (Lian et al., 2014)
Hippuric acid	5	24	Free chlorine	HA5
Hippuric acid	30	170	Free chlorine, TCM	HA30

Supporting information S2 - Chlorine demand: experimental results

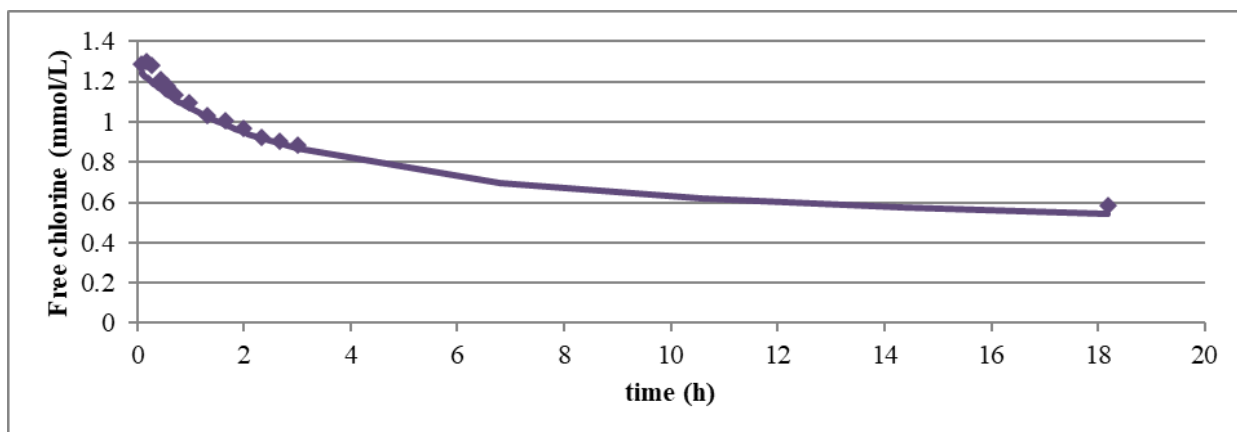


Figure S 1 Chlorine demand from urea chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

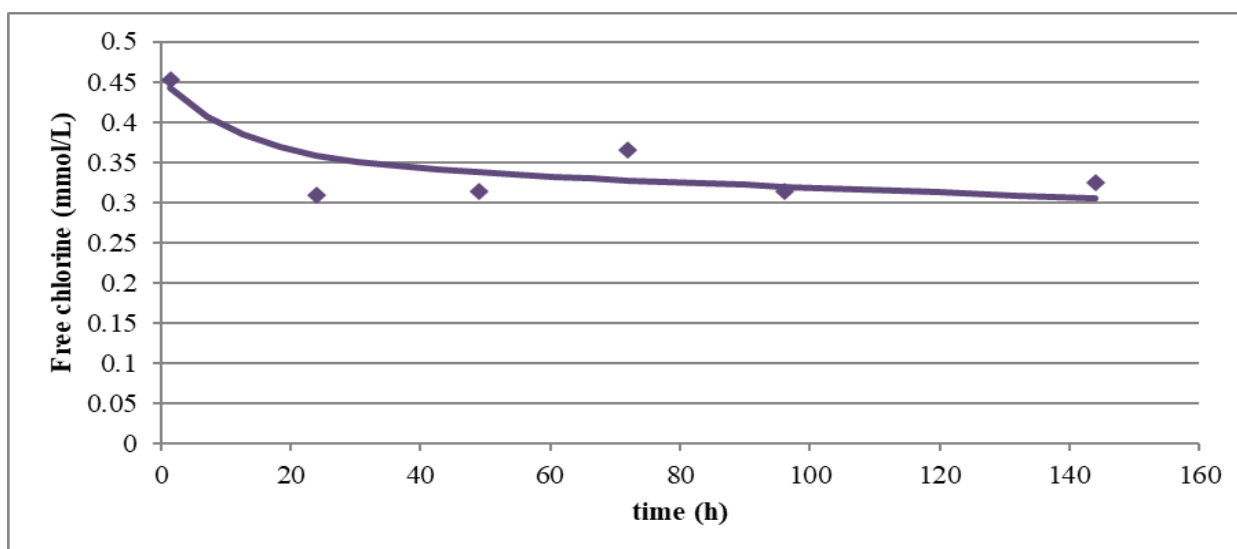


Figure S 2 Chlorine demand from creatinine chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

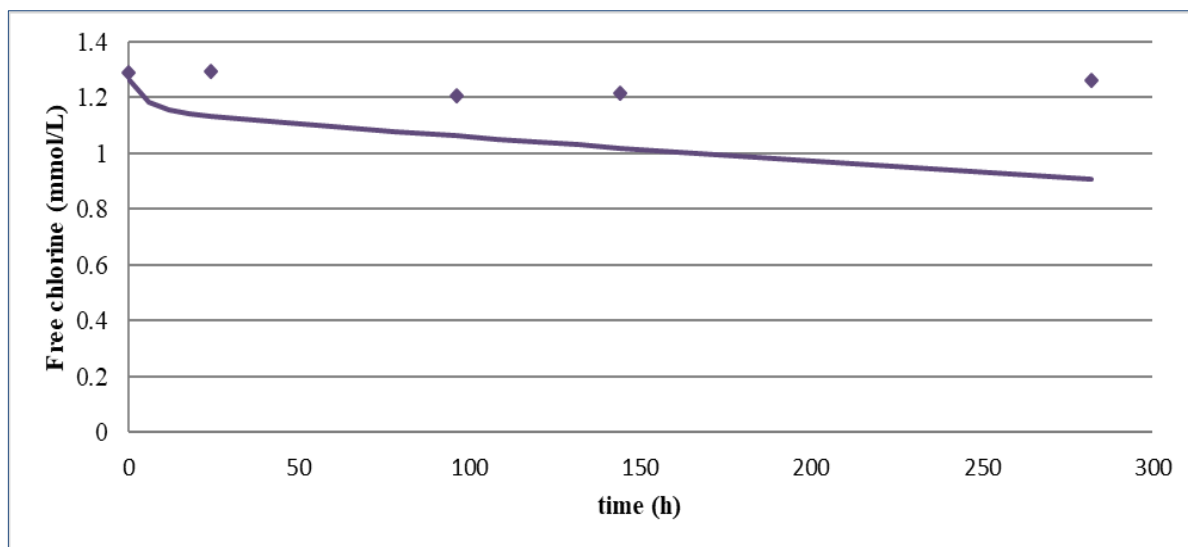


Figure S 3 Chlorine demand from creatinine chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

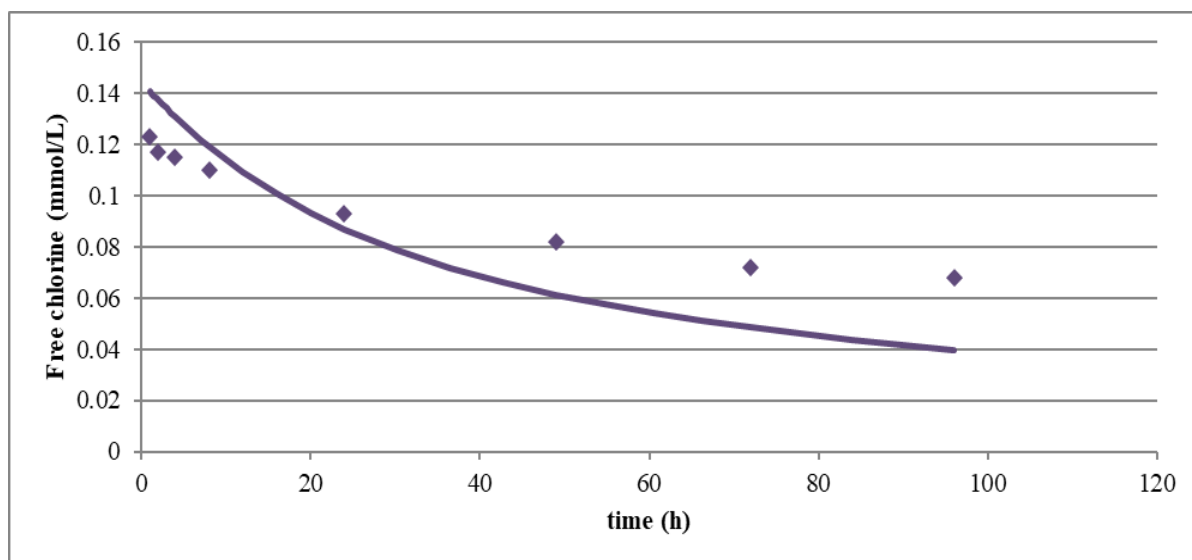


Figure S 4 Chlorine demand from creatinine chlorination, $[Cl_2]_0 = 10$ ppm, $[creatinine]_0 = 18 \mu M$ (Li et al., 2007)

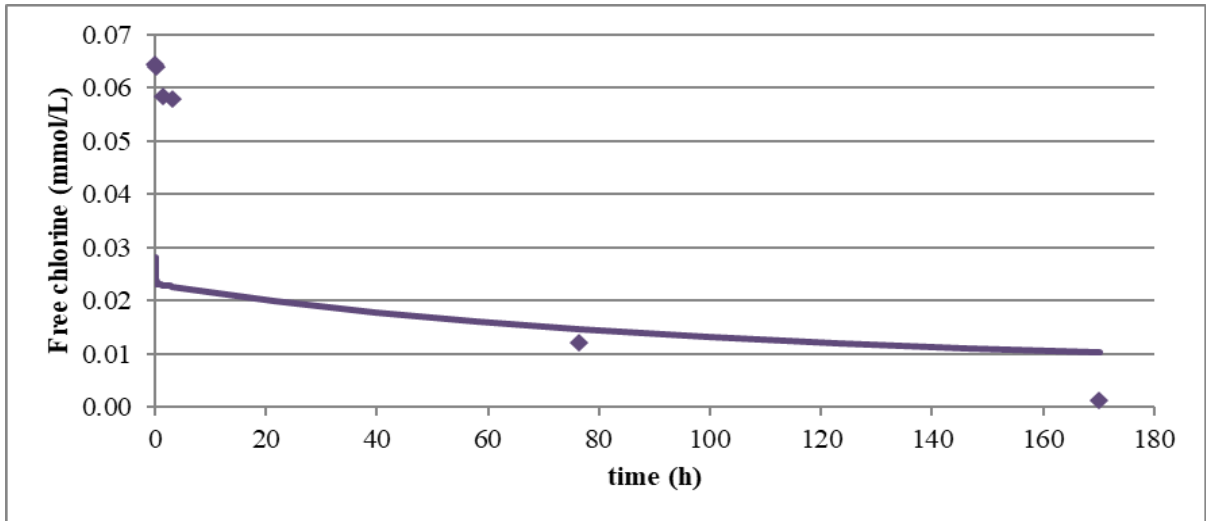


Figure S 5 Chlorine demand from L-histidine chlorination, $[Cl_2]_0 = 5$ ppm, $T = 27^\circ C$

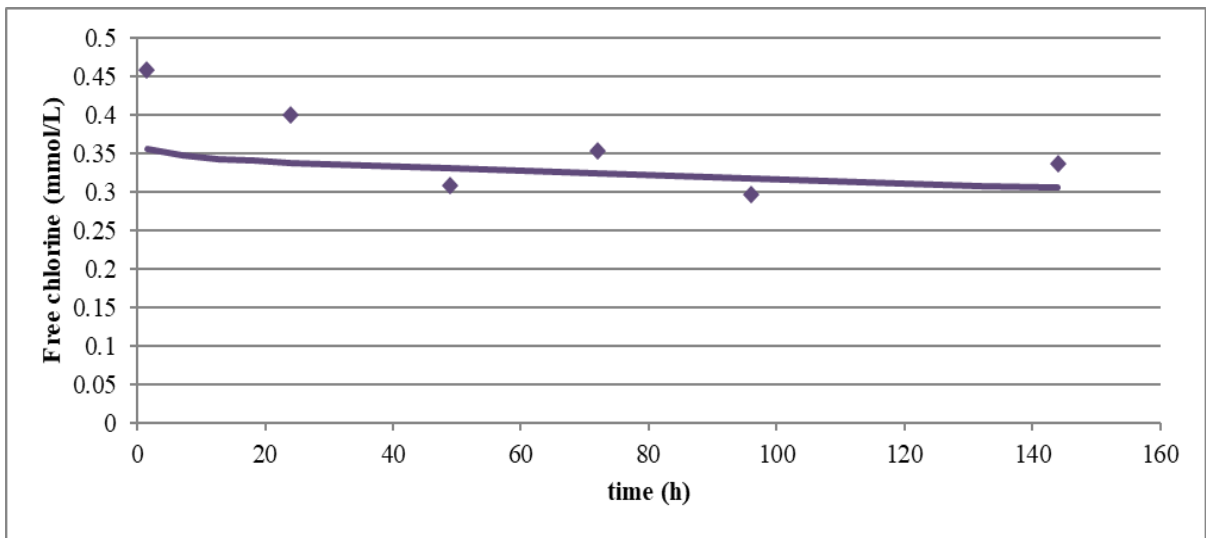


Figure S 6 Chlorine demand from L-histidine chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

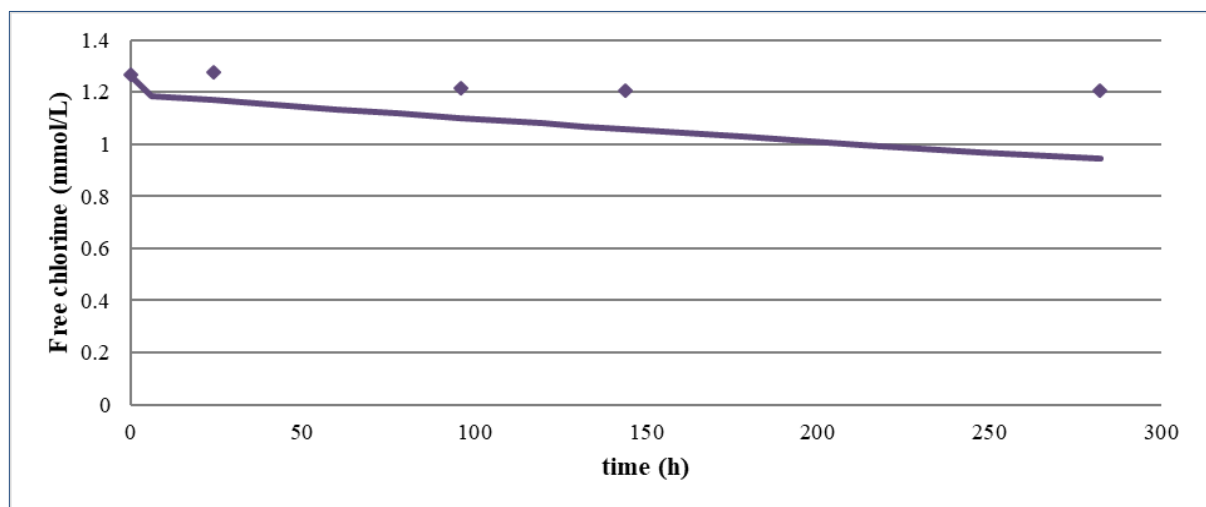


Figure S 7 Chlorine demand from L-histidine chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

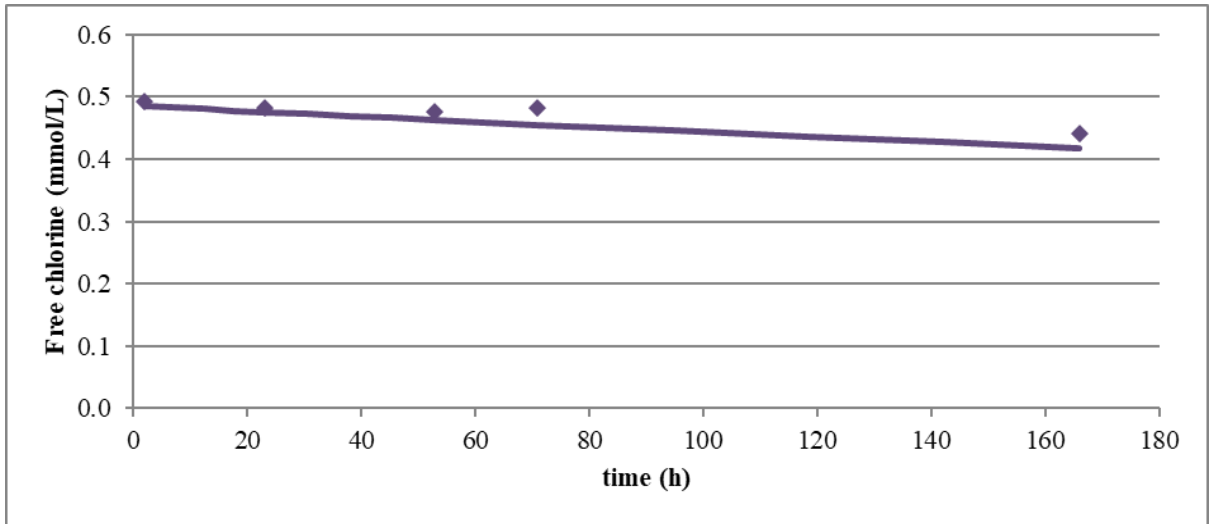


Figure S 8 Chlorine demand from citric acid chlorination, $[\text{Cl}_2]_0 = 30 \text{ ppm}$, $T = 27^\circ\text{C}$

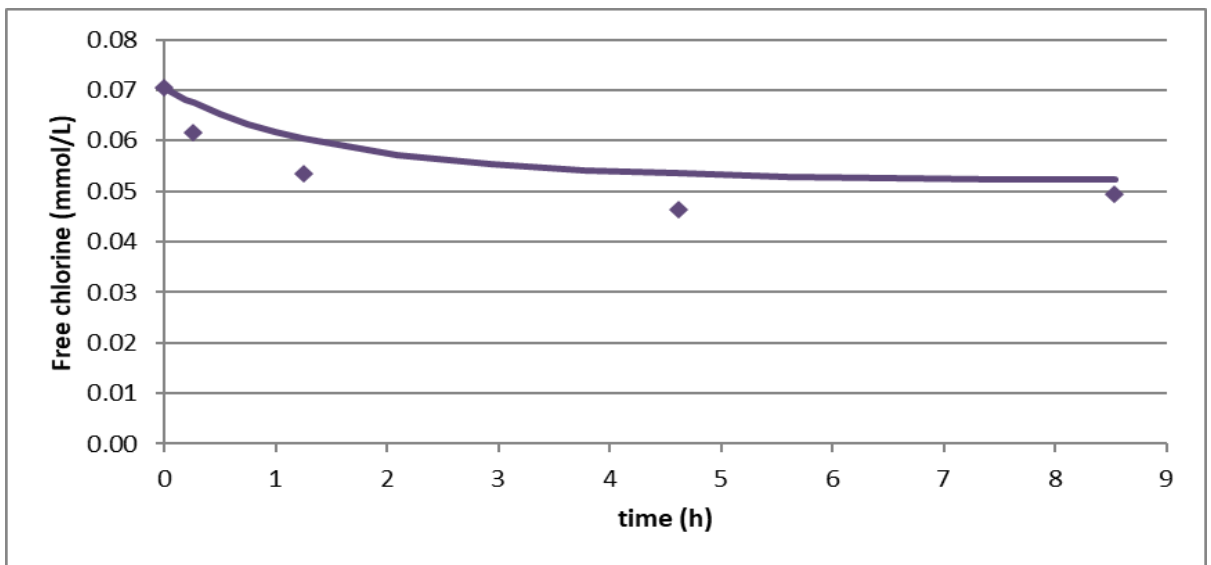


Figure S 9 Chlorine demand from uric acid chlorination, $[\text{Cl}_2]_0 = 5 \text{ ppm}$, $T = 27^\circ\text{C}$

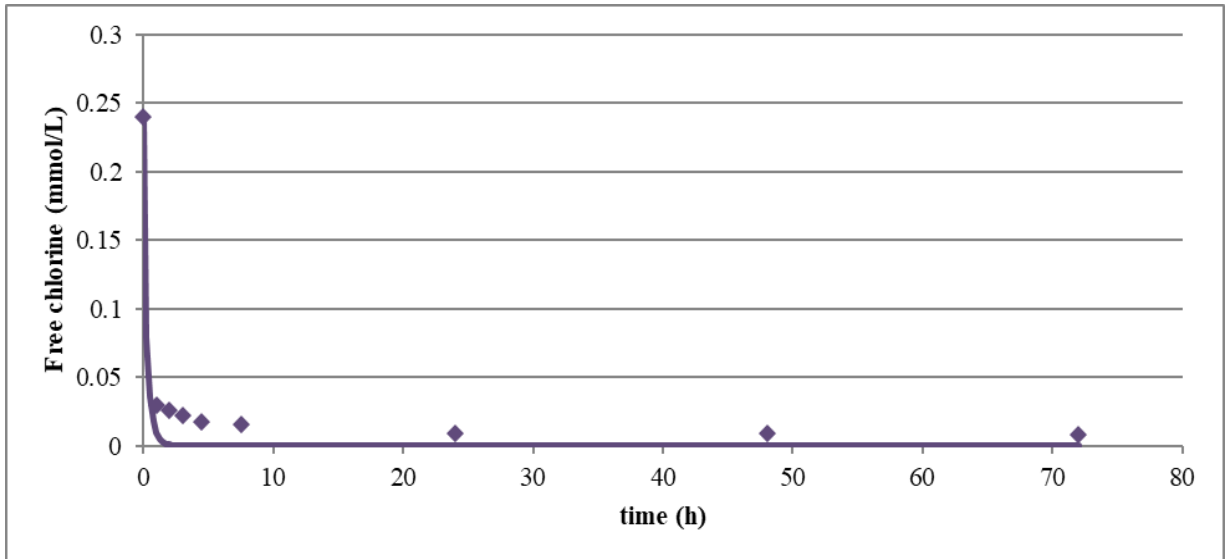


Figure S 10 Chlorine demand from uric acid chlorination, $[Cl_2]_0 = 17$ ppm, $[uric\ acid]_0 = 50$ μ M, pH = 7 (Lian et al., 2014)

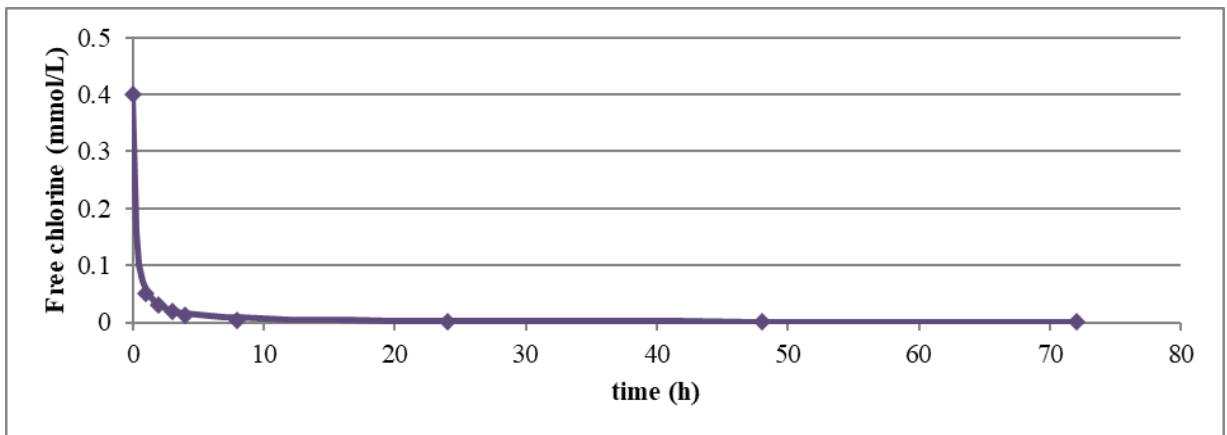


Figure S 11 Chlorine demand from uric acid chlorination, $[Cl_2]_0 = 28$ ppm, $[uric\ acid]_0 = 50$ μ M, pH = 7 (Lian et al., 2014)

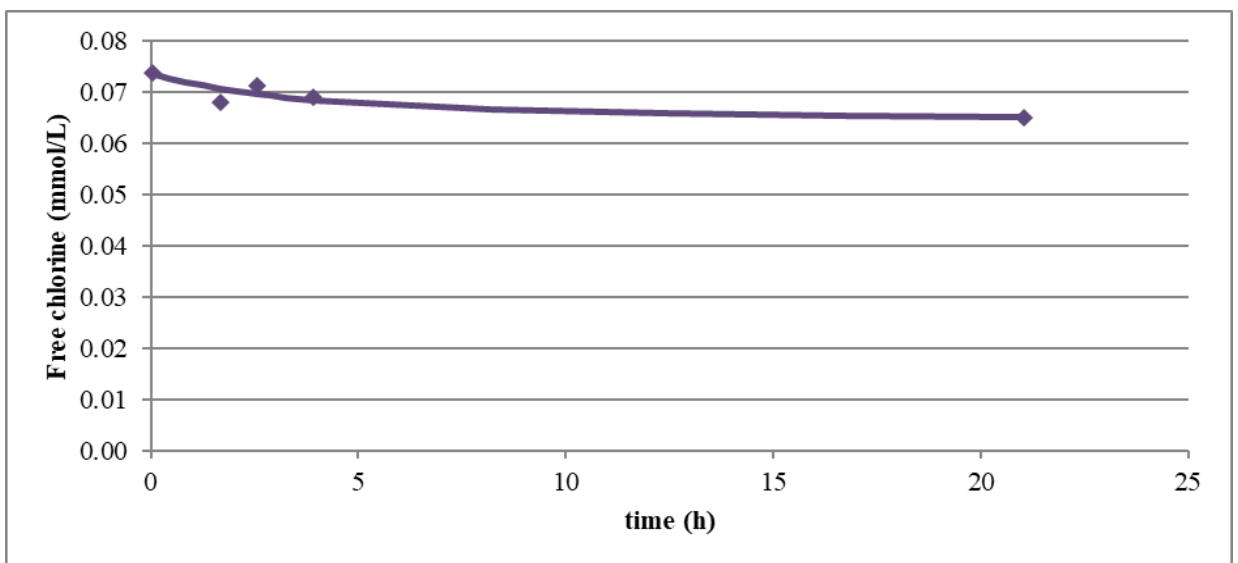


Figure S 12 Chlorine demand from hippuric acid chlorination, $[Cl_2]_0 = 5$ ppm, T = 27°C

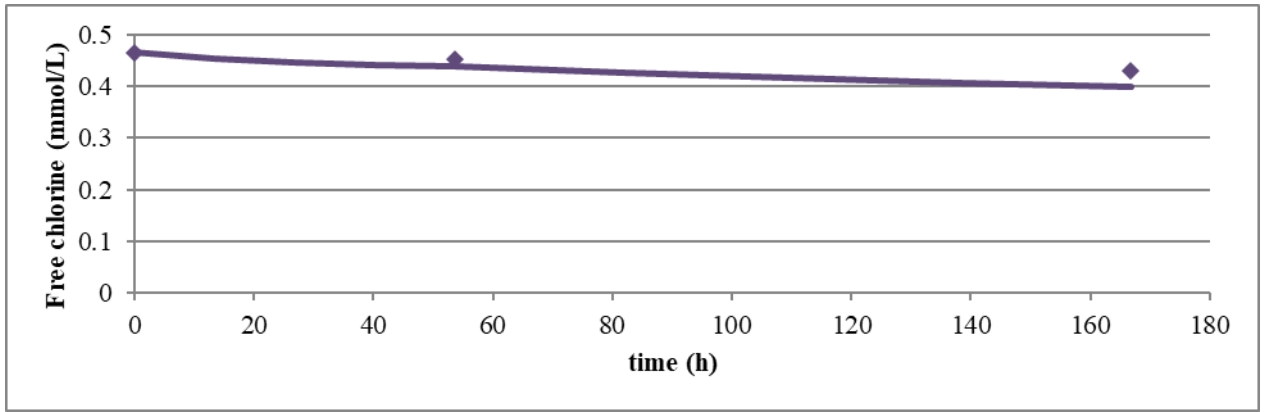


Figure S 13 Chlorine demand from hippuric acid chlorination, $[\text{Cl}_2]_0 = 30 \text{ ppm}$, $T = 27^\circ\text{C}$

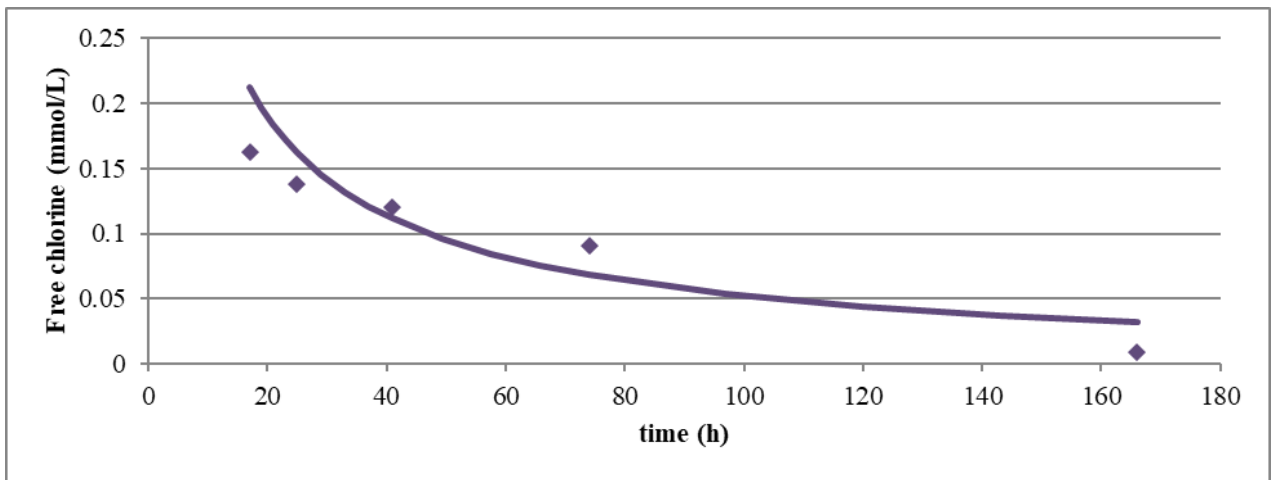


Figure S 14 Chlorine demand from BFA chlorination, $[\text{Cl}_2]_0 = 65 \text{ ppm}$, $T = 27^\circ\text{C}$

Supporting information S3 - Chloroform formation: experimental results

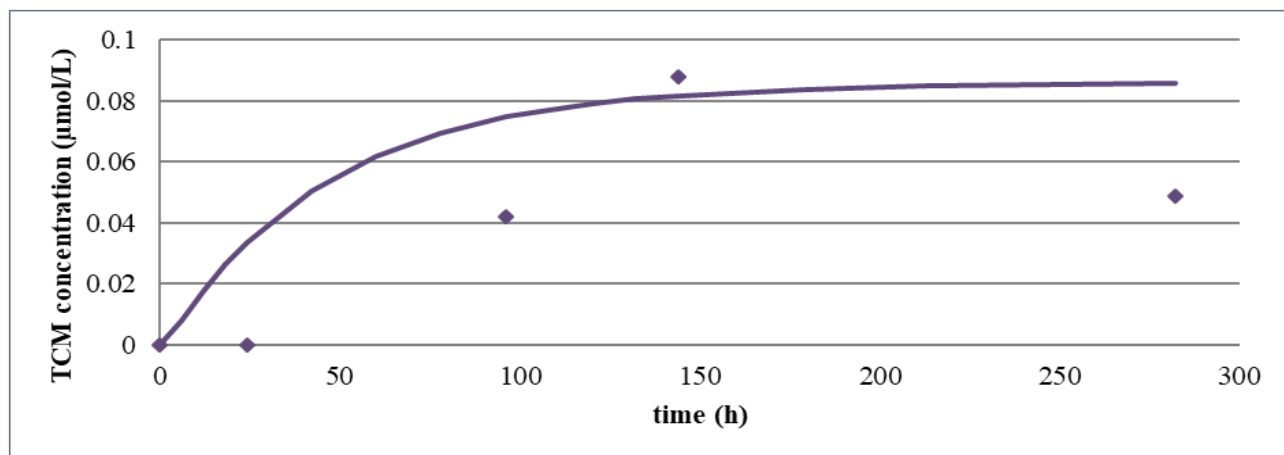


Figure S 15 TCM formation from creatinine chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

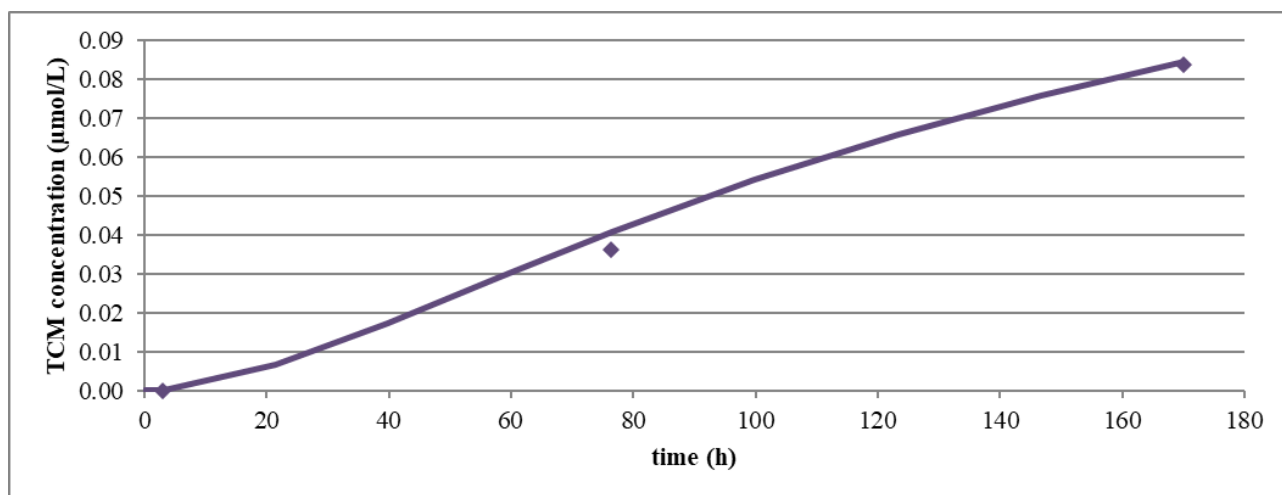


Figure S 16 TCM formation from L-histidine chlorination, $[Cl_2]_0 = 5$ ppm, $T = 27^\circ C$

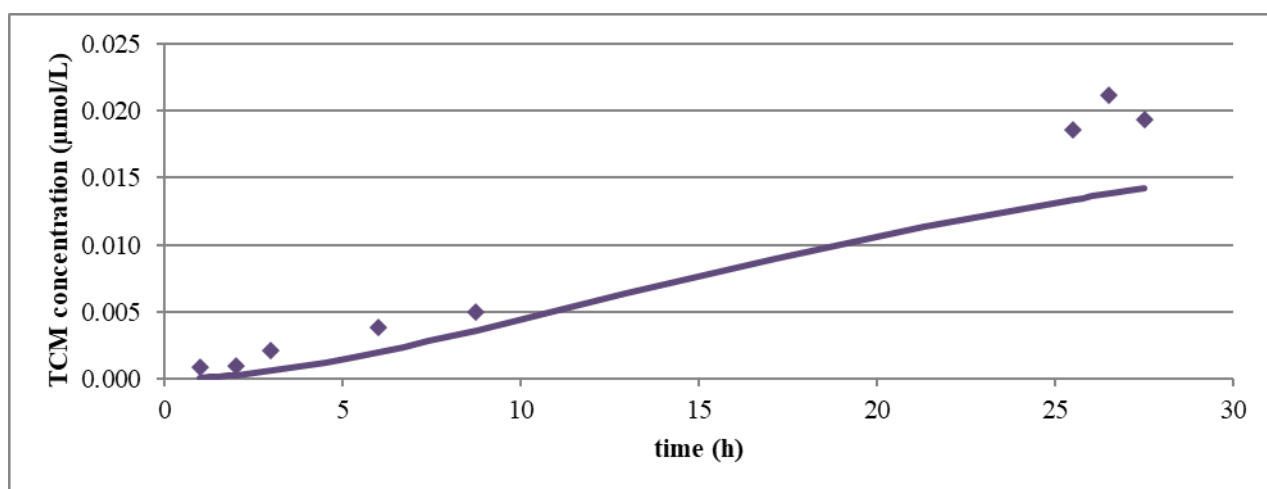


Figure S 17 TCM formation from L-histidine chlorination, $[Cl_2]_0 = 10$ ppm, $T = 27^\circ C$

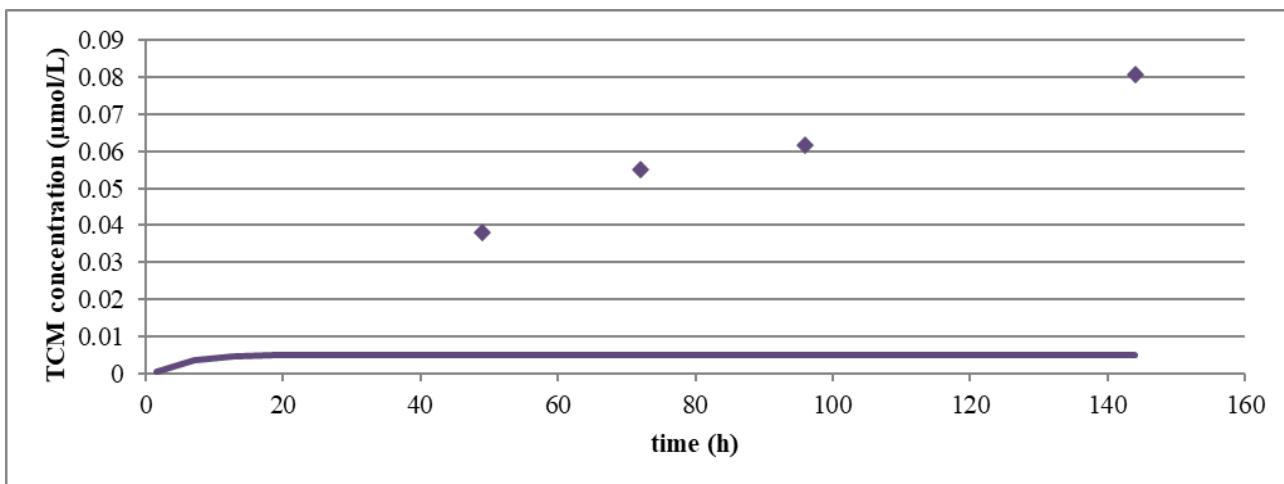


Figure S 18 TCM formation from L-histidine chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

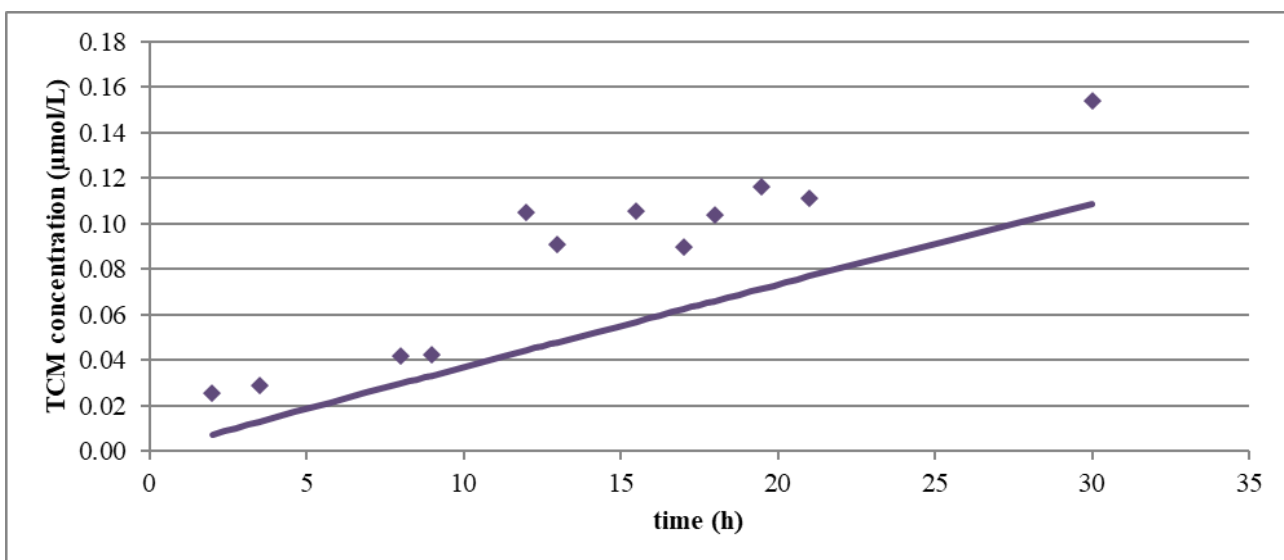


Figure S 19 TCM formation from citric acid chlorination, $[Cl_2]_0 = 10$ ppm, $T = 27^\circ C$

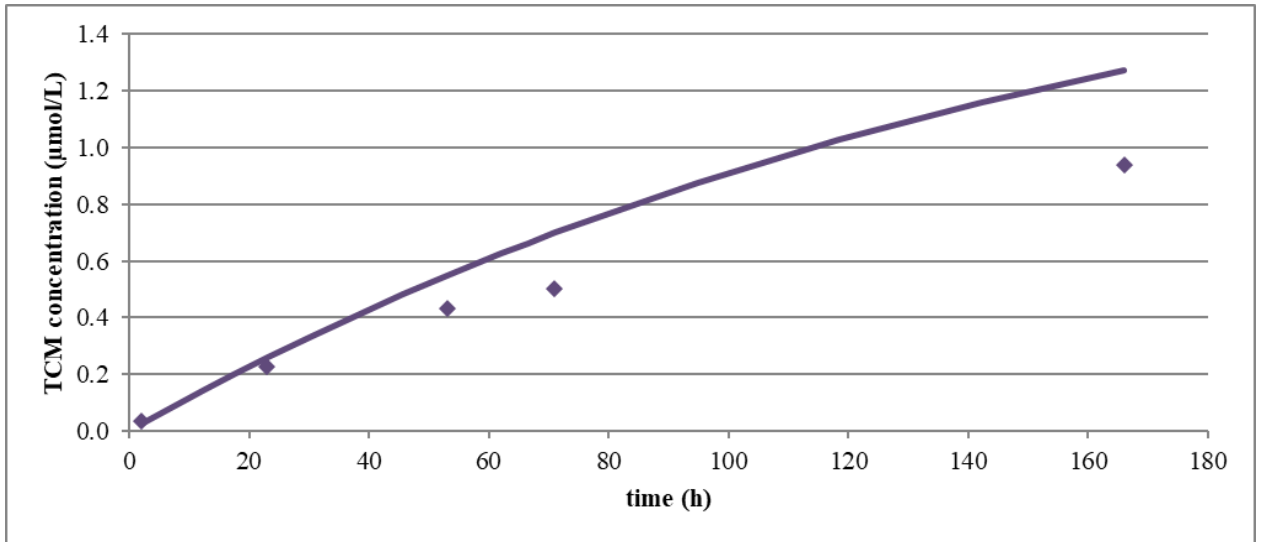


Figure S 20 TCM formation from citric acid chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

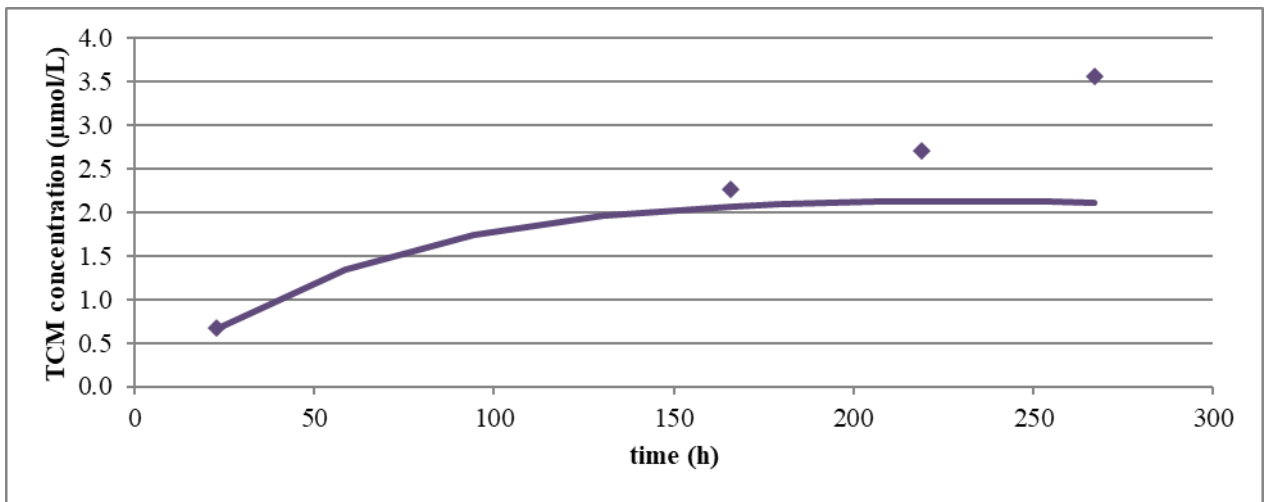


Figure S 21 TCM formation from citric acid chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

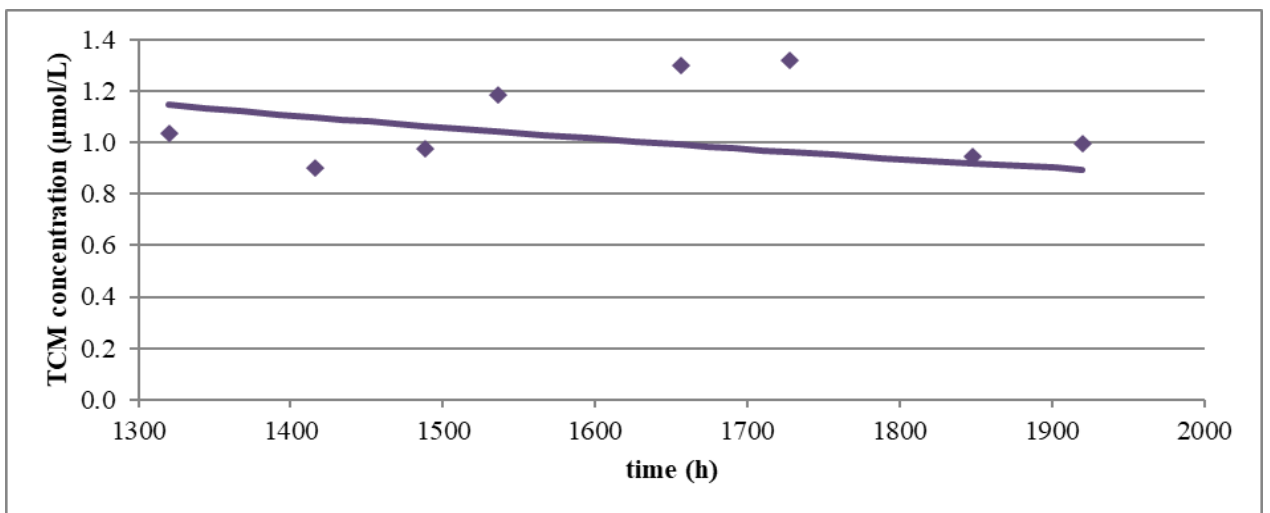


Figure S 22 TCM formation from citric acid chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

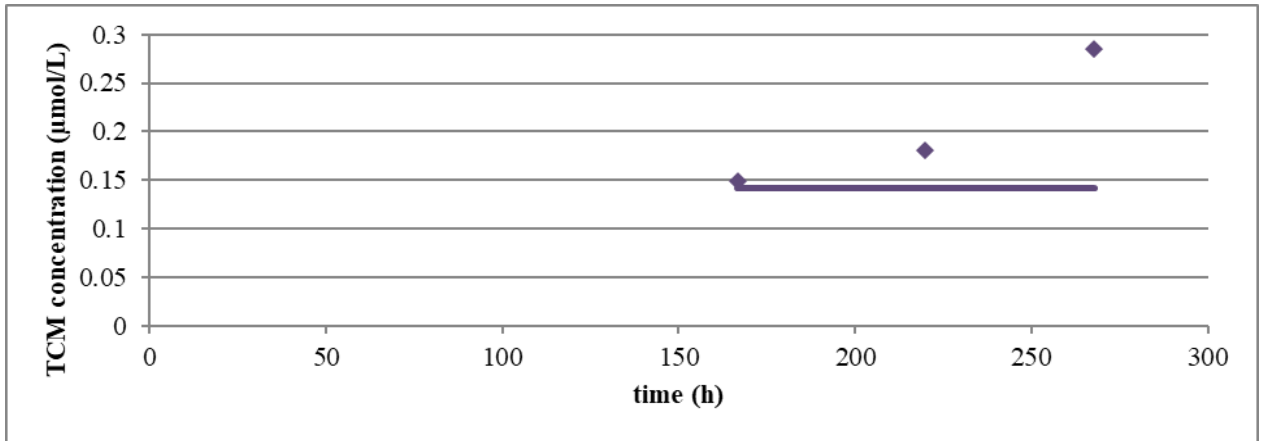


Figure S 23 TCM formation from uric acid chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

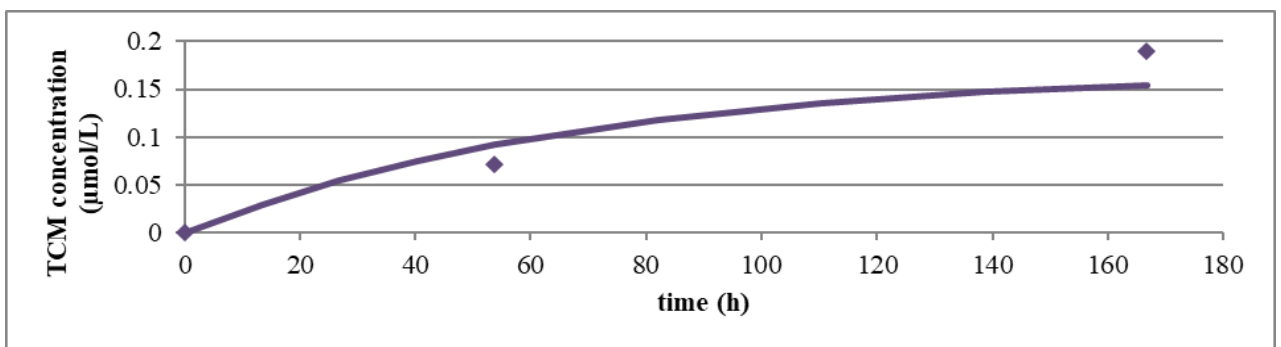


Figure S 24 TCM formation from hippuric acid chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

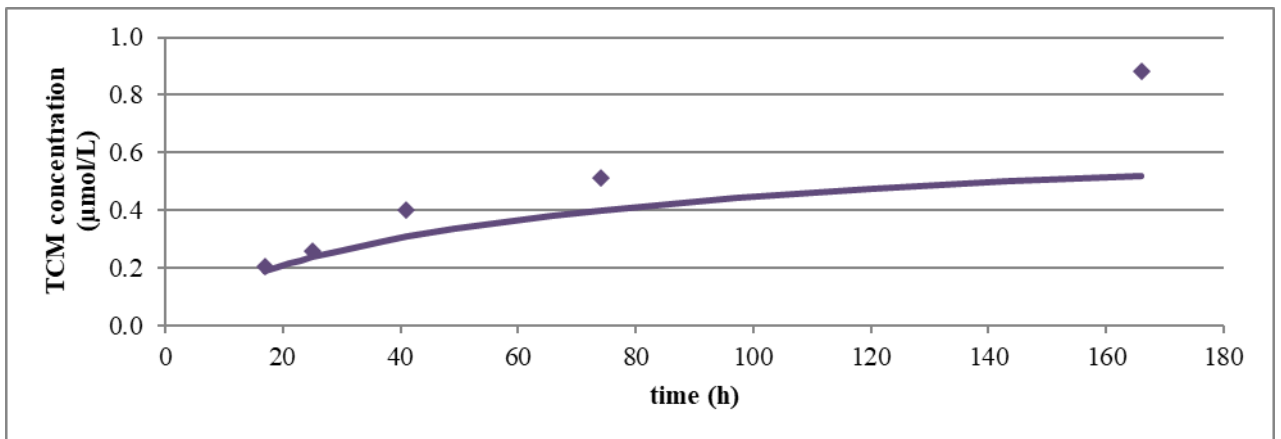


Figure S 25 TCM formation from BFA chlorination, $[Cl_2]_0 = 65$ ppm, $T = 27^\circ C$

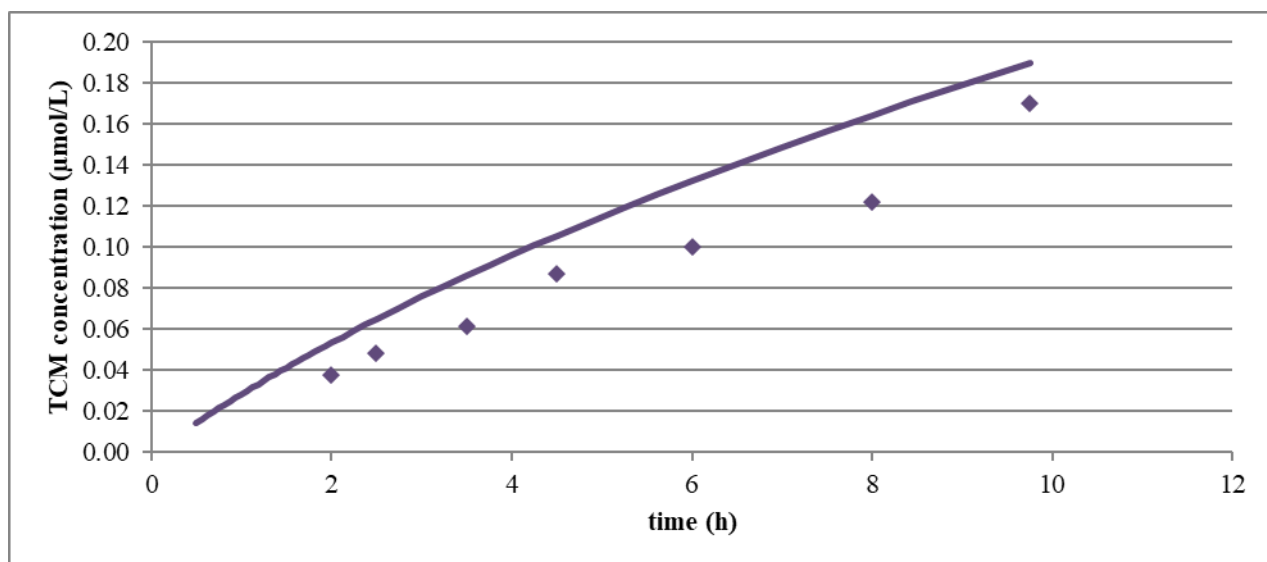


Figure S 26 TCM formation from BFA chlorination, $[Cl_2]_0 = 90$ ppm, $T = 27^\circ C$

Supporting information S4 – Chlorination mechanisms

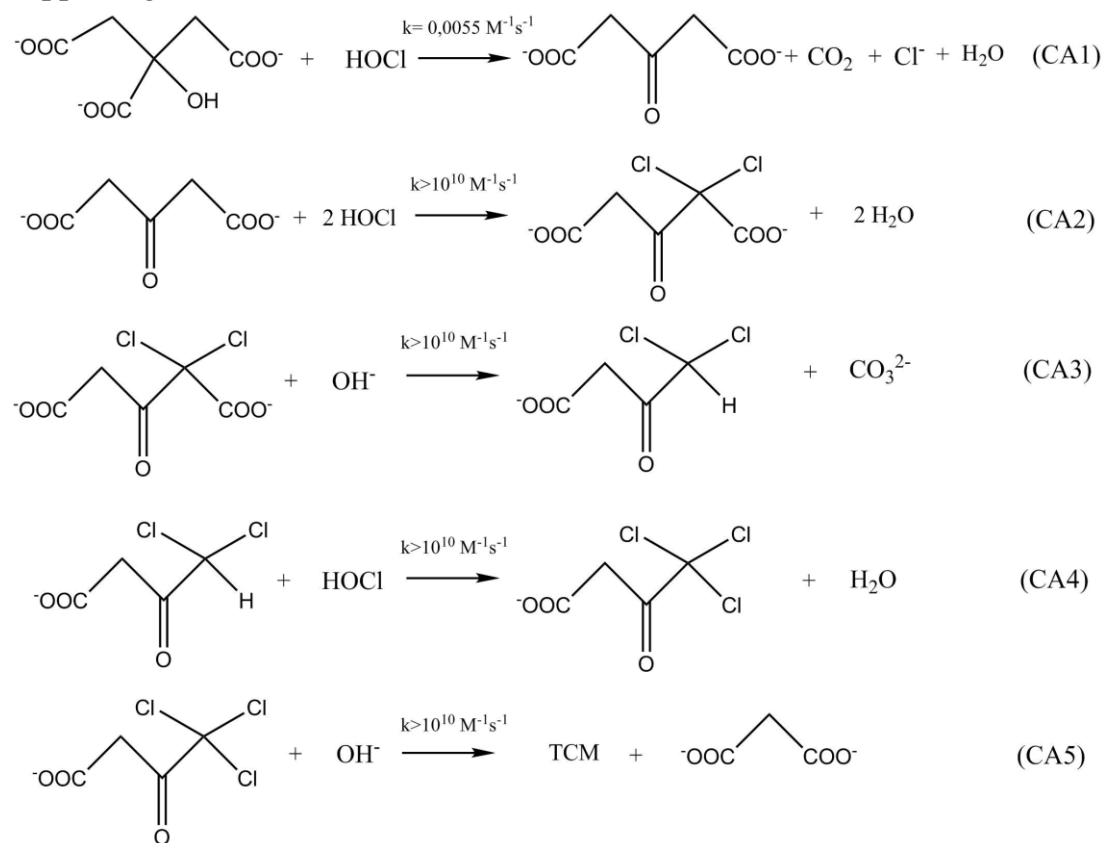


Figure S 27 TCM formation from citric acid chlorination

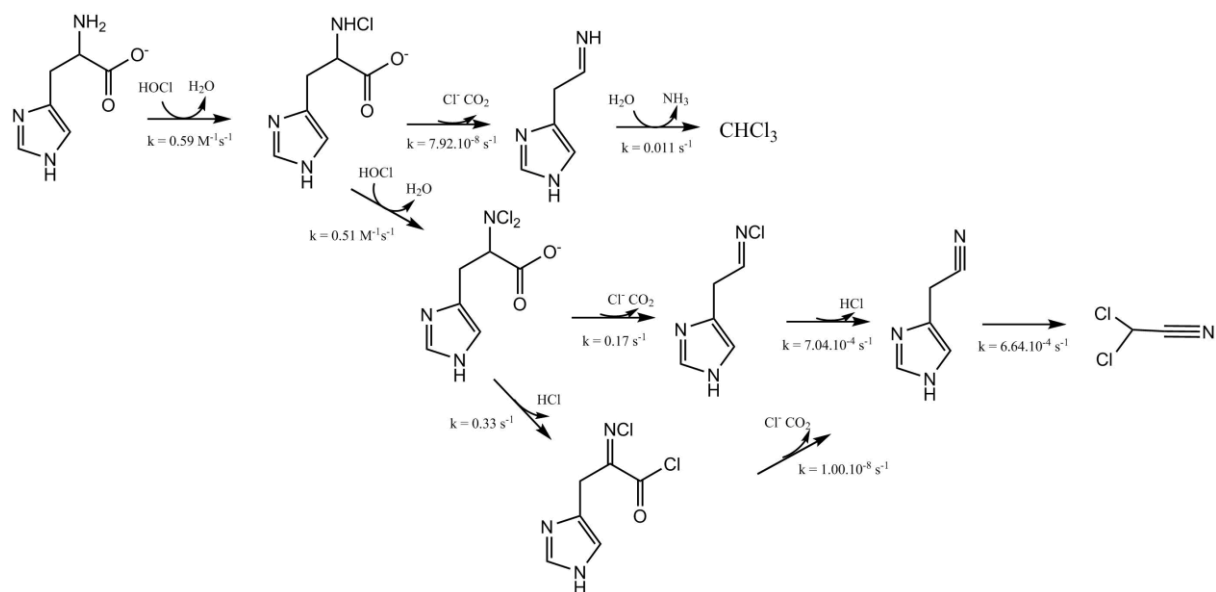


Figure S 28 DCAN formation from L-histidine chlorination, with kinetic rates obtained in this study (Li et al., 2017)

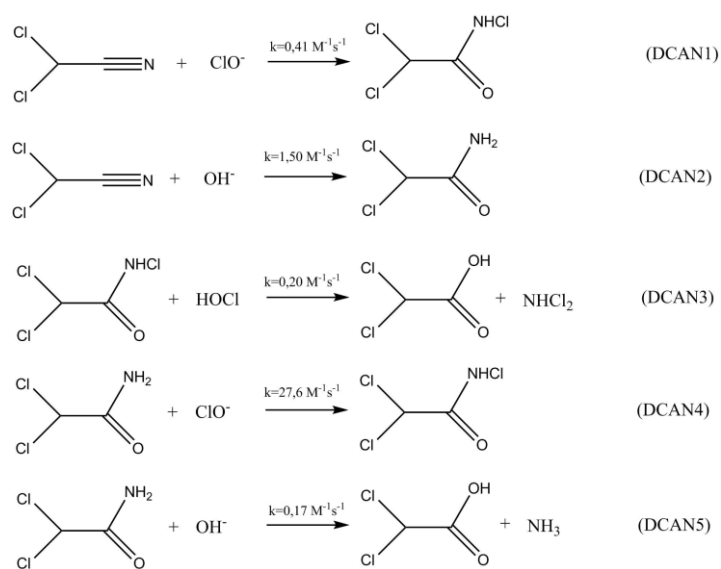


Figure S 29 Degradation mechanism of DCAN by reaction with ClO^- and OH^- as reported by Yu and Reckhow (Yu and Reckhow, 2017)

Supporting information S5 – Dichloroacetonitrile and dichloromethylamine formation: experimental results

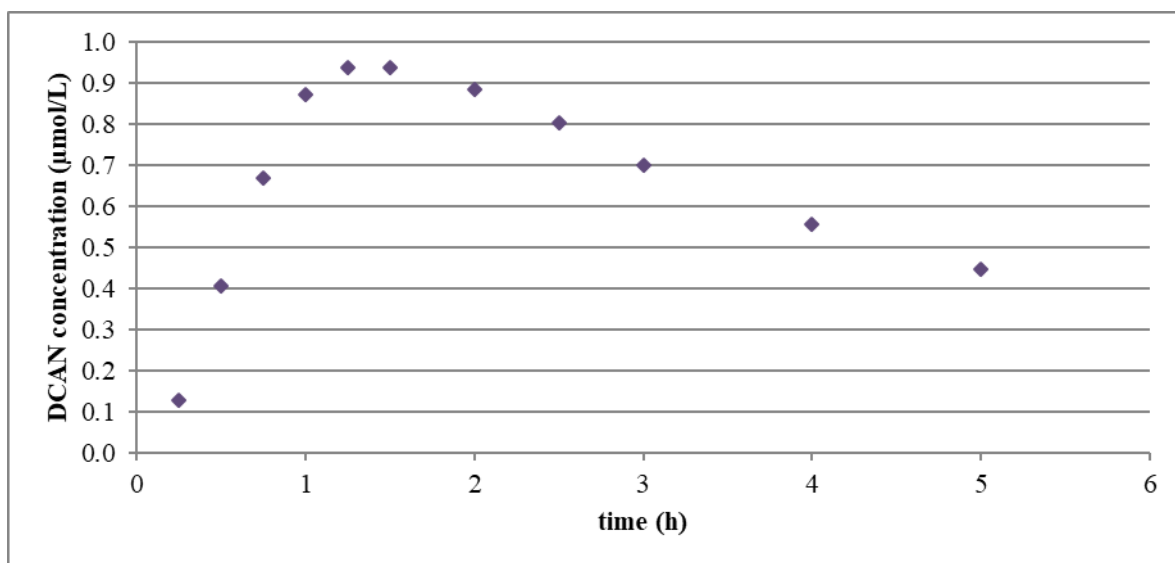


Figure S 30 DCAN formation from BFA chlorination, $[\text{Cl}_2]_0 = 90$ ppm, $T = 27^\circ\text{C}$

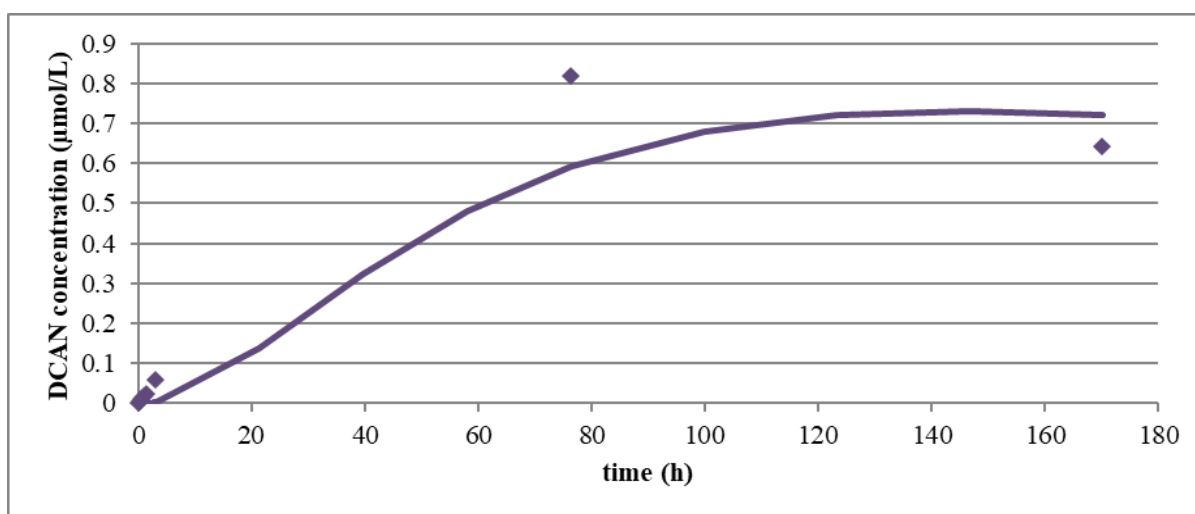


Figure S 31 DCAN formation from L-histidine chlorination, $[\text{Cl}_2]_0 = 5$ ppm, $T = 27^\circ\text{C}$

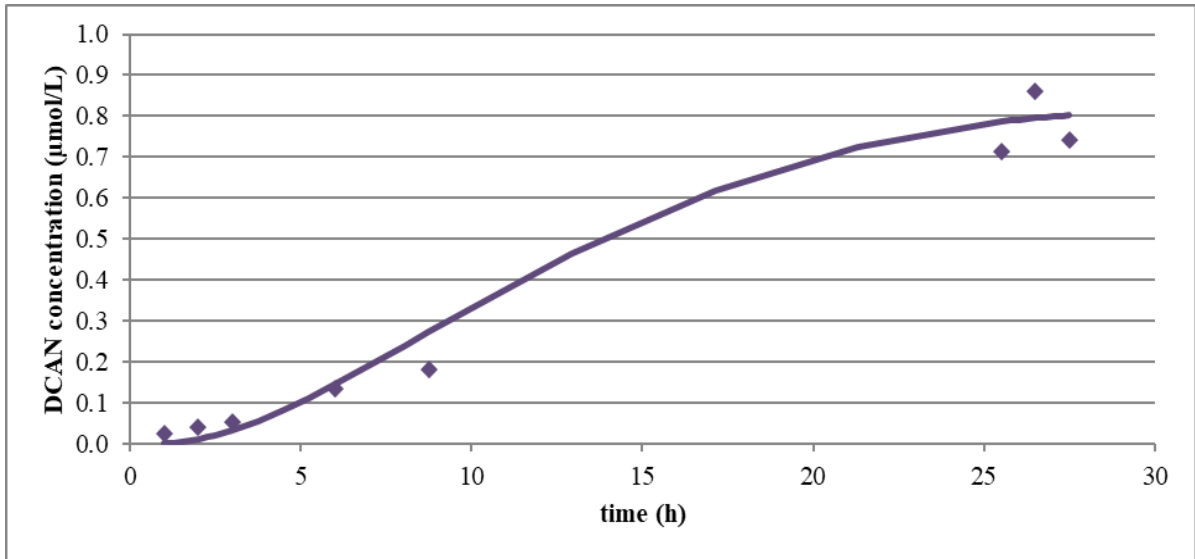


Figure S 32 DCAN formation from L-histidine chlorination, $[Cl_2]_0 = 10$ ppm, $T = 27^\circ C$

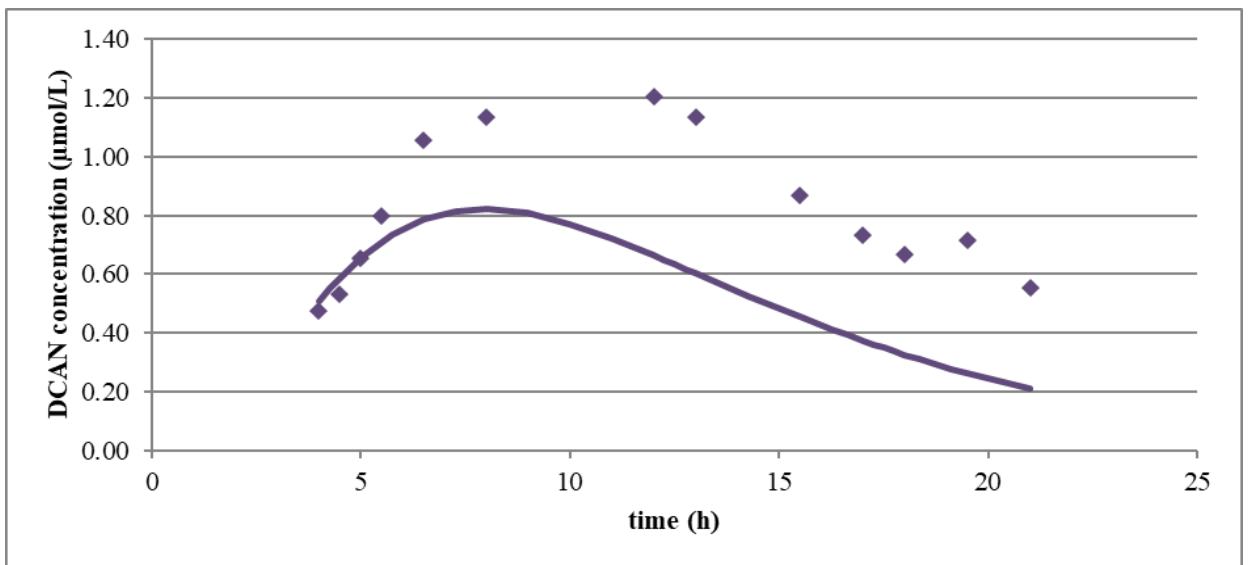


Figure S 33 DCAN formation from L-histidine chlorination, $[Cl_2]_0 = 30$ ppm, $T = 27^\circ C$

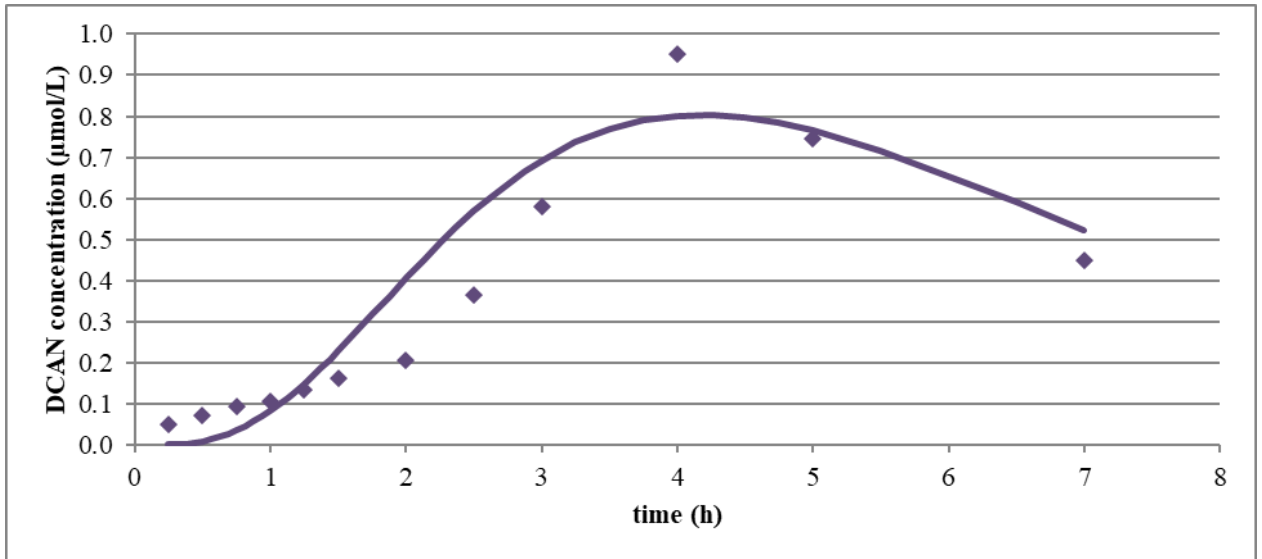


Figure S 34 DCAN formation from L-histidine chlorination, $[\text{Cl}_2]_0 = 60 \text{ ppm}$, $T = 27^\circ\text{C}$

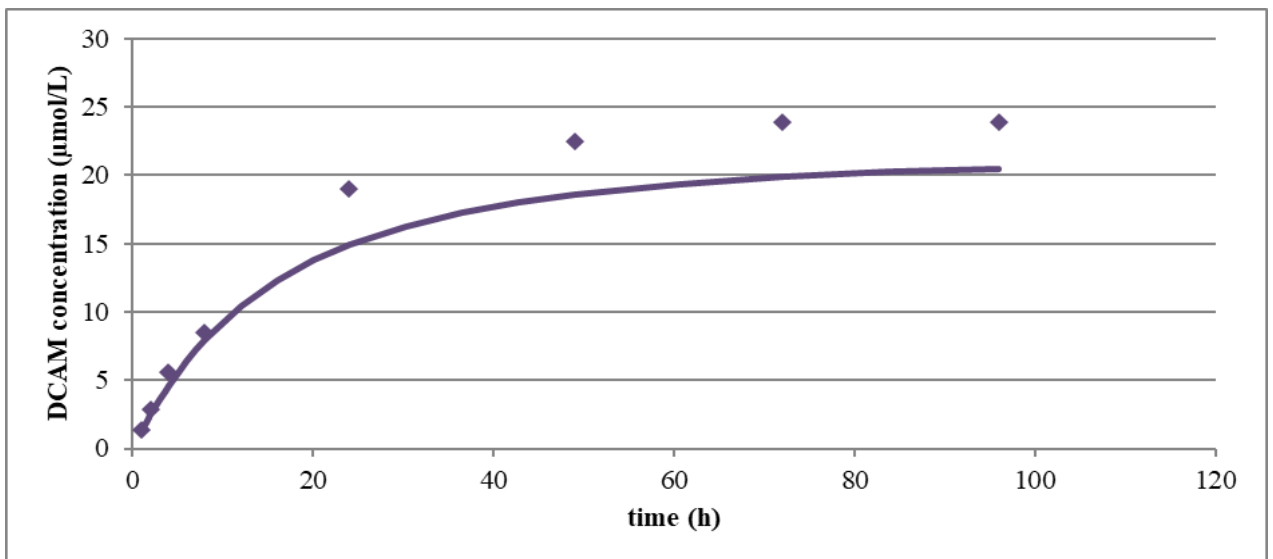


Figure S 35 DCMA formation from creatinine chlorination, $[\text{Cl}_2]_0 = 10 \text{ ppm}$, $[\text{creatinine}]_0 = 18 \mu\text{M}$ (Li et al., 2007)