Supporting Information

Formation of disinfection byproducts in wash water and lettuce by washing with sodium hypochlorite and peracetic acid sanitizers

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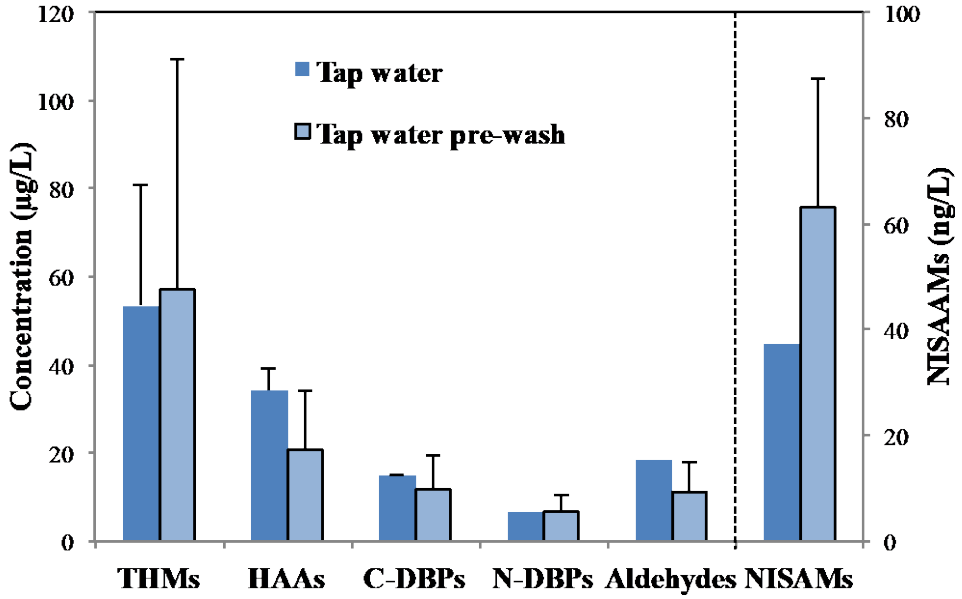

Figure S1. DBPs levels in the original tap water (n = 2) and in the "pre-wash" water sample generated after pre-washing lettuce by tap water for 10 min (n = 4).

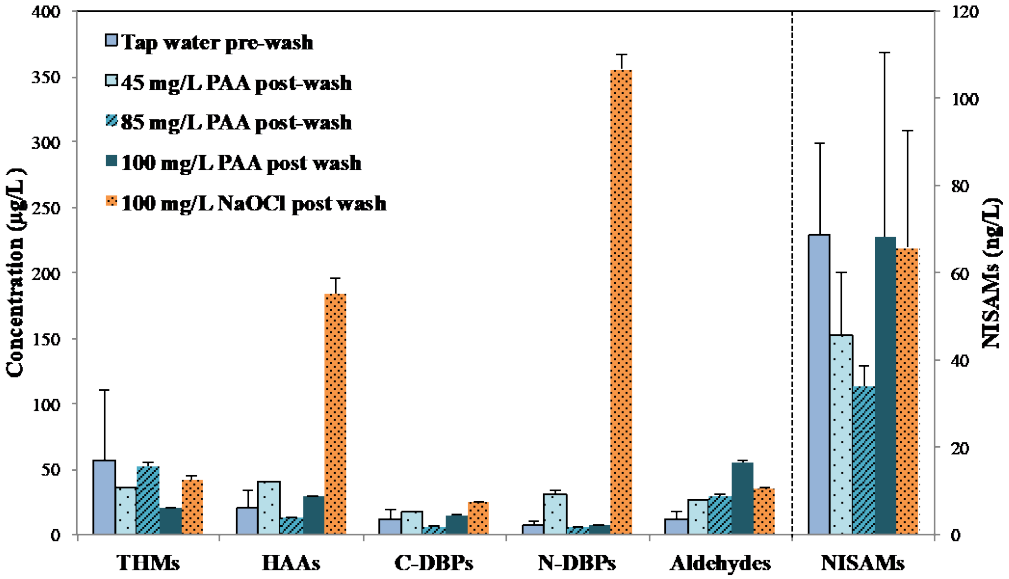

Figure S2. Concentrations of DBPs in the wash water from tap water pre-wash of fresh-cut lettuce (n = 4), and tap water post-wash from different sanitizer washes (n = 2 for each experiment).

Table S1. Retention time, recovery and MDL in lettuce wash water and lettuce for five target aldehydes (n = 8).

Aldehydes	Retention Time (RSD%) (min)	**Lettuce Wash Water**		**Lettuce**	
		Recovery (RSD%) (%)	MDL (μg/L)	Recovery (RSD%) (%)	MDL (ng/g)
FD	16.78 (0.04)	185 (7.2)	0.65	205 (7.4)	9.03
AD	20.43 (0.00)	241 (2.3)	1.88	249 (1.0)	1.48
BD	39.57 (0.02)	176 (1.0)	1.79	53 (0.3)	0.10
GX	45.17 (0.00), 45.32 (0.01)	162 (5.4)	0.13	193 (10.6)	0.80
MG	45.32 (0.01), 45.78 (0.00)	152 (0.2)	0.47	52 (3.9)	1.21

Table S2. Recovery and estimated MDL in lettuce for six target nitrosamines (n = 3).

NISAMs	Recovery (RSD%) (%)	Estimated MDL (ng/g)
NDMA	26 (8.4)	0.1
NMEA	52 (3.0)	0.25
NDEA	81 (2.1)	0.1
NDPA	82 (2.7)	0.1
NMOR	52 (5.2)	0.1
NPYR	57 (3.6)	0.1

Table S3. Concentrations of DBPs in wash water after washing fresh-cut lettuce. Wash water samples included tap water **pre-wash** (20 °C) and then **sanitizer wash** (PAA or NaOCl, 5 °C, pH 6). ND = non-detectable.

DBP Group	DBP compound	Pre-wash (by tap water)	PAA 45 mg/L	PAA 85 mg/L	PAA 100 mg/L	NaOCl 100 mg/L
THMs (μg/L)	CF	**48.5±51.7**	**49.4±0.54**	**63.6±1.09**	**3.39±0.56**	**25.0±4.90**
	BF	<MDL	<MDL	<MDL	<MDL	<MDL
	BDCM	7.55±0.77	0.13±0.002	0.16±0.01	0.02±0.01	0.24±0.06
	DBCM	1.08±0.15	ND	ND	ND	0.18±0.01
	Total	57.1±52.4	49.6±0.55	63.8±1.08	3.41±0.55	25.4±4.96
HAAs (μg/L)	MCAA	0.69±0.56	0.26±0.04	0.24±0.002	0.38±0.04	1.97±0.11
	MBAA	0.19	<MDL	<MDL	0.28±0.01	0.41±0.04
	DCAA	7.13±6.05	0.70±0.008	0.31±0.008	0.41±0.02	**83.1±0.54**
	TCAA	**9.84±5.47**	**0.89±0.001**	**0.54±0.05**	**0.72±0.03**	36.1±0.28
	BCAA	1.33±1.09	0.30±0.002	<MDL	0.28±0.02	13.7±0.24
	DBAA	<MDL	<MDL	<MDL	<MDL	5.13±0.001
	BDCAA	1.17±0.66	<MDL	<MDL	<MDL	31.1±1.13
	CDBAA	ND	ND	ND	ND	6.06±0.32
	TBAA	0.75±0.33	<MDL	<MDL	<MDL	44.7±1.94
	Total	21.0±13.2	2.16±0.05	1.09±0.04	2.08±0.11	222±2.27
C-DBPs (μg/L)	CH	**9.48±6.18**	**<MDL**	<MDL	**0.24±0.04**	**36.2±0.36**
	DCPN	0.48±0.19	ND	ND	ND	1.93±0.32
	TCPN	1.06±0.82	ND	ND	ND	7.86±0.78
	TetraCPN	ND	ND	ND	ND	0.67
	PentaCPN	ND	ND	ND	ND	1.74±0.26
	DBCPN	<MDL	ND	**<MDL**	<MDL	<MDL
	TriCE	ND	ND	ND	ND	0.97±0.31
	TCE	ND	ND	ND	ND	ND
	TCEL	ND	ND	ND	ND	ND
	CTC	<MDL	ND	ND	ND	ND
	DBE	1.08±0.91	<MDL	ND	ND	0.41
	Total	11.9±7.55	<MDL	<MDL	<MDL	49.2±2.07
N-DBPs (μg/L)	BNM	ND	ND	<MDL	<MDL	<MDL
	TCNM	0.30±0.19	**0.15±0.00**	**0.16±0.001**	0.15±0.004	0.35±0.03
	DCAN	1.67±0.76	<MDL	ND	ND	**79.8±8.42**
	TCAN	<MDL	ND	ND	ND	0.61±0.23
	BCAN	0.50±0.11	ND	ND	ND	3.31±0.17
	DBAN	<MDL	<MDL	<MDL	<MDL	<MDL
	DCAAm	**3.56±3.26**	ND	ND	**0.32±0.03**	50.0±3.01
	TCAAm	0.78±0.02	ND	ND	<MDL	10.6±1.22
	Total	6.68±4.20	0.15±0.00	0.20±0.004	0.47±0.03	145±6.20
NISAMs (ng/L)	NDMA	ND	ND	ND	ND	ND
	NMEA	ND	ND	ND	ND	ND
	NDEA	<MDL	<MDL	<MDL	<MDL	<MDL
	NDPA	ND	ND	ND	ND	ND
	NMOR	ND	ND	ND	ND	ND
	NPYR	ND	ND	ND	ND	ND
	NPIP	**56.9±17.4**	**66.5±0.99**	**42.9±1.66**	**53.0±7.02**	**47.8±14.7**
	NDBA	11.8±3.85	ND	ND	40.8±12.4	ND
	Total	68.7±20.8	66.5±0.99	42.9±1.66	93.7±19.4	47.8±14.7
Aldehydes (μg/L)	FD	**4.18±5.74**	**63.2±1.36**	**82.9±6.38**	**86.4±0.75**	18.8±0.04
	AD	3.93±2.61	4.47±0.32	4.54±0.49	5.31±0.19	**107±2.66**
	BD	<MDL	ND	ND	<MDL	<MDL
	GX	2.25±1.04	5.51±0.03	8.15±0.81	6.77±0.26	8.07±0.17
	MG	2.84±2.65	<MDL	<MDL	<MDL	0.74±0.04
	Total	11.0±6.67	73.2±1.64	95.5±6.70	98.5±0.82	134±2.58

Table S4. Concentrations (**in ng DBP/g lettuce**) of DBPs in **fresh-cut lettuce** with or without washing. The washing included tap water pre-wash (20 °C), then sanitizer wash (PAA, or NaOCl, 5 °C, pH 6), and final tap water post-wash (20 °C). ND = non-detectable.

DBP Group	DBP compound	Lettuce Background	PAA 45 mg/L	PAA 85 mg/L	PAA 100 mg/L	NaOCl 100 mg/L
THMs	CF	**91.6**	**145±3.93**	**126±8.23**	**242±23.4**	**490±217**
	BF	ND	ND	ND	ND	ND
	BDCM	ND	ND	ND	ND	ND
	DBCM	ND	ND	ND	ND	ND
	Total	91.6	145±3.93	126±8.23	242±23.4	490±217
HAAs	MCAA	**21.7**	**11.0±8.70**	**9.90±4.81**	**12.2±8.70**	13.5±0.59
	MBAA	ND	ND	ND	ND	8.09±0.49
	DCAA	1.00	6.41±0.06	1.92±0.03	3.00±0.17	**354±19.4**
	TCAA	4.93	5.87±0.09	6.09±0.38	5.54±0.35	61.3±3.79
	BCAA	ND	3.75±3.94	7.57±4.08	ND	4.95±0.53
	DBAA	ND	ND	ND	ND	<MDL
	BDCAA	ND	ND	ND	ND	4.00±0.06
	CDBAA	<MDL	ND	ND	<MDL	<MDL
	TBAA	<MDL	ND	ND	<MDL	ND
	Total	27.6	27.1±12.5	25.5±9.24	20.7±9.23	445±23.6
C-DBPs	CH	ND	<MDL	<MDL	**3.77±0.07**	22.7±9.15
	DCPN	ND	<MDL	<MDL	<MDL	**37.3±17.1**
	TCPN	ND	ND	ND	ND	6.85±3.59
	TetraCPN	ND	ND	ND	ND	24.3±10.4
	PentaCPN	ND	ND	ND	ND	ND
	DBCPN	**<MDL**	**3.15±0.19**	**3.35±0.14**	2.82	4.00±1.70
	TriCE	ND	ND	ND	ND	ND
	TCE	ND	ND	ND	ND	ND
	TCEL	ND	ND	ND	ND	ND
	CTC	ND	ND	ND	<MDL	ND
	DBE	ND	ND	ND	ND	ND
	Total	<MDL	3.15±0.19	3.35±0.14	5.18±1.92	95.2±41.9
N-DBPs	BNM	ND	ND	ND	ND	ND
	TCNM	ND	ND	ND	ND	ND
	DCAN	ND	ND	ND	ND	<MDL
	TCAN	ND	ND	ND	ND	ND
	BCAN	ND	ND	ND	ND	ND
	DBAN	ND	<MDL	<MDL	<MDL	ND
	DCAAm	**53.7**	**14.7±0.02**	**15.3±2.02**	**15.2±1.15**	**61.6±6.93**
	TCAAm	ND	ND	ND	ND	<MDL
	Total	53.7	14.7±0.02	15.3±2.02	15.2±1.15	61.6±6.93
NISAMs	NDMA	0.18	0.19	**0.43±0.21**	**0.39±0.02**	0.22±0.06
	NMEA	ND	ND	ND	ND	ND
	NDEA	ND	<MDL	0.18±0.21	<MDL	<MDL
	NDPA	ND	ND	ND	ND	ND
	NMOR	**2.29**	ND	ND	ND	**0.74**
	NPYR	ND	ND	ND	ND	ND
	Total	2.47	0.19	0.62±0.00	0.39±0.02	0.22±0.06
Aldehydes	FD	21.5	38.7±0.79	42.5±0.76	35.9±4.44	43.8±5.57
	AD	**94.9**	**137±2.70**	**136±0.51**	**124±9.48**	**106±5.43**
	BD	2.34	1.64±0.04	1.66±0.04	0.89±0.16	1.36±00.28
	GX	29.9	7.33±0.34	9.94±0.53	6.60±1.06	12.4±0.18
	MG	6.87	1.87±0.15	2.55±0.17	2.09±0.33	3.44±0.08
	Total	155	186±2.45	192±1.93	170±15.5	167±0.70

Table S5. Concentrations of DBPs in the **post-wash** water samples. The post-wash samples were from tap water (20 °C) washing lettuce that was washed by different sanitizer solutions. ND = non-detectable.

DBP Group	DBP compound	PAA 45 mg/L	PAA 85 mg/L	PAA 100 mg/L	NaOCl 100 mg/L
THMs (μg/L)	CF	**27.8±0.27**	**42.4±2.88**	**11.9±0.21**	**30.4±3.07**
	BF	<MDL	<MDL	<MDL	<MDL
	BDCM	6.79±0.07	8.10±0.19	7.66±0.13	9.57±0.68
	DBCM	1.09±0.02	1.27±0.01	0.99±0.02	1.48±0.04
	Total	35.6±0.33	51.7±3.08	20.5±0.37	41.4±3.80
HAAs (μg/L)	MCAA	1.61±0.07	0.60±0.01	1.13±0.14	1.72±0.02
	MBAA	0.19±0.02	<MDL	<MDL	0.27±0.002
	DCAA	**19.1±0.15**	3.62±0.10	9.96±0.21	**154±12.1**
	TCAA	13.6±0.44	**6.35±0.33**	**12.6±0.36**	20.7±0.26
	BCAA	3.06±0.10	0.86±0.002	2.00±0.08	4.30±0.01
	DBAA	0.32±0.01	<MDL	<MDL	0.38±0.001
	BDCAA	1.86±0.03	0.84±0.02	1.56±0.11	2.18±0.08
	CDBAA	ND	ND	ND	ND
	TBAA	0.76±0.01	0.74±0.04	1.13±0.001	0.71±0.13
	Total	40.5±0.79	13.0±0.51	28.4±0.90	184±12.6
C-DBPs (μg/L)	CH	**10.2±0.19**	**4.30±0.14**	**12.7±0.25**	**10.7±0.36**
	DCPN	0.92±0.01	0.61±0.01	<MDL	1.17±0.07
	TCPN	3.41±0.004	0.91±0.001	0.95±0.003	4.92±0.20
	TetraCPN	<MDL	ND	ND	5.73±1.04
	PentaCPN	ND	ND	ND	ND
	DBCPN	<MDL	ND	ND	<MDL
	TriCE	ND	ND	ND	ND
	TCE	ND	ND	ND	ND
	TCEL	<MDL	ND	ND	ND
	CTC	ND	<MDL	ND	ND
	DBE	2.95±0.07	0.57±0.02	1.42±0.03	1.72±0.06
	Total	17.5±0.27	6.39±0.15	15.0±0.28	24.3±1.07
N-DBPs (μg/L)	BNM	ND	ND	ND	ND
	TCNM	0.56±0.01	0.22±0.02	0.52±0.02	0.44±0.04
	DCAN	2.31±0.01	1.26±0.001	1.99±0.02	11.0±0.08
	TCAN	ND	ND	ND	ND
	BCAN	0.69±0.004	0.17±0.02	0.52±0.01	1.01±0.03
	DBAN	<MDL	<MDL	<MDL	<MDL
	DCAAm	**26.9±1.91**	**3.58±0.45**	**3.22±0.33**	**338±10.9**
	TCAAm	0.54±0.07	0.74±0.03	0.81±0.01	4.91±0.83
	Total	31.0±2.01	5.96±0.39	7.04±0.31	355±11.6
NISAMs (ng/L)	NDMA	ND	ND	ND	27.5
	NMEA	ND	ND	ND	ND
	NDEA	<MDL	<MDL	15.1	<MDL
	NDPA	ND	ND	ND	ND
	NMOR	ND	ND	ND	ND
	NPYR	ND	ND	ND	ND
	NPIP	**45.6±14.4**	**33.9±4.86**	**52.8±20.2**	**45.3±36.9**
	NDBA	<MDL	<MDL	11.6±6.01	13.4
	Total	45.6±14.4	33.9±4.86	68.3±42.0	65.8±26.8
Aldehydes (μg/L)	FD	**12.8±0.18**	**11.7±0.005**	**27.3±0.26**	11.6±2.10
	AD	12.1±0.06	11.6±0.60	22.1±0.95	**19.6±0.10**
	BD	<MDL	<MDL	<MDL	<MDL
	GX	0.82±0.13	5.97±0.08	5.95±0.01	2.51±0.06
	MG	ND	<MDL	<MDL	0.79±0.005
	Total	25.8±0.37	29.2±0.69	55.3±1.22	34.5±2.26