

Triclosan

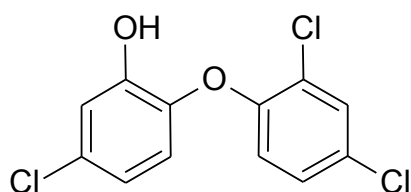
BMF 82 - Triclosan

Impurities and degradation products

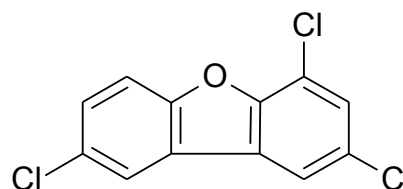
Triclosan (5-Chloro-2-(2,4-dichlorophenoxy)phenol; Cat. No. 8472.12) is an antimicrobial agent extensively used in soaps, shampoos, deodorants, toothpaste etc. and the content typically varies from 0.1-1%.

Triclosan is a white crystalline substance with structural similarities to dibenzo-p-dioxins and dibenzofurans. Its mechanisms of action, risk of bacterial resistance and its possible role in disruption of hormonal development has been controversial.

Our interest in triclosan increased following purification of a commercial sample by repeated crystallizations, which yielded the PCDF 2,4,8-trichlorodibenzofuran (Cat. No. 11789.12) rather than triclosan itself.



Triclosan
(Cat. No. 8472.12)



2,4,8-Trichlorodibenzofuran
(Cat. No. 11789.12)

Triclosan reacts with free chlorine in tap water to produce reduced amounts of other compounds, like 2,4-dichlorophenol. Some of these compounds convert into dioxins upon exposure by UV-radiation.¹ However, the dioxins that can form from triclosan are not considered to be congeners of toxicological concern for mammals, birds and fish.²⁻⁴



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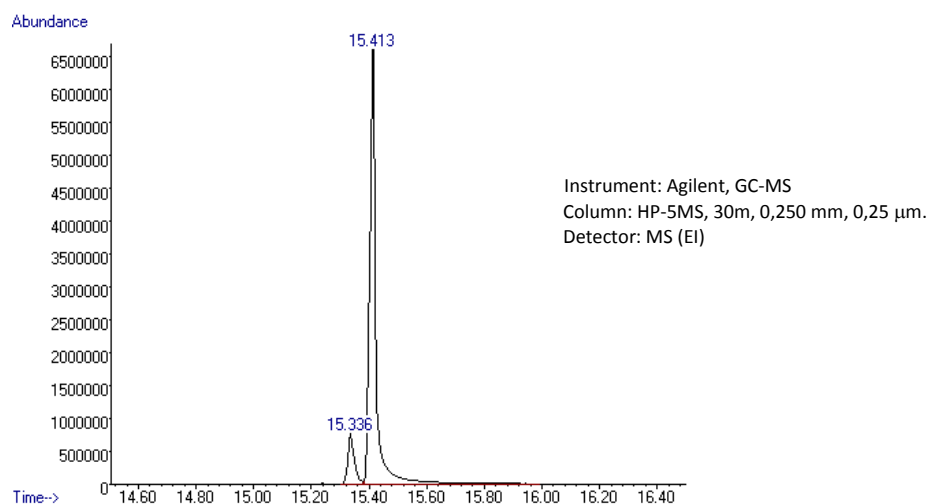
The following organic impurities may be found in commercial triclosan samples:

Table 1. Impurities of triclosan⁵

Individual related compounds (GC)	≤ 0.1%
Total related compounds (GC)	≤ 0.5%
2,4-Dichlorophenol	≤ 10 mg/kg
Sum of 3- and 4-Chlorophenol	≤ 10 mg/kg
2,3,7,8-Tetrachlorodibenzo- <i>p</i> -dioxin	< 0.001 µg/kg
2,3,7,8-Tetrachlorodibenzofuran	< 0.001 µg/kg
2,8-Dichlorodibenzo- <i>p</i> -dioxin	≤ 0.5 mg/kg
1,3,7-Trichlorodibenzo- <i>p</i> -dioxin	≤ 0.25 mg/kg
2,8-Dichlorodibenzofuran	≤ 0.25 mg/kg
2,4,8-Trichlorodibenzofuran	≤ 0.5 mg/kg

We analysed the content of 2,4,8-trichlorodibenzofuran (Cat. No. 11789.12) in a commercial triclosan sample, and found it to be present in the order of 10%, raising the question of lack of quality control of commercial household products.

Figure 1: GC-MS of commercial triclosan sample



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Figure 2: Mass spectrum of triclosan (Cat.No 8447.12)
Retention time 15.413

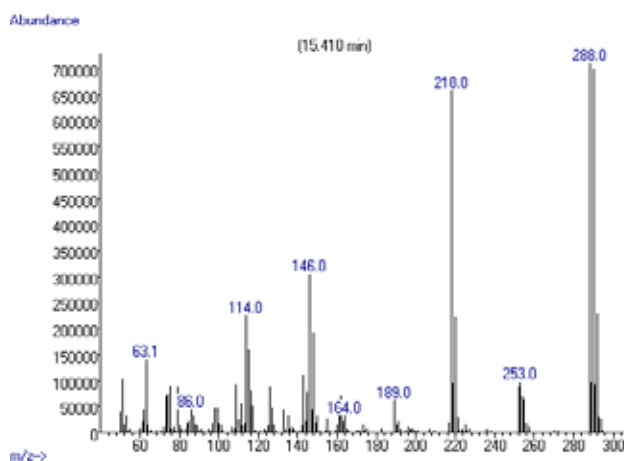
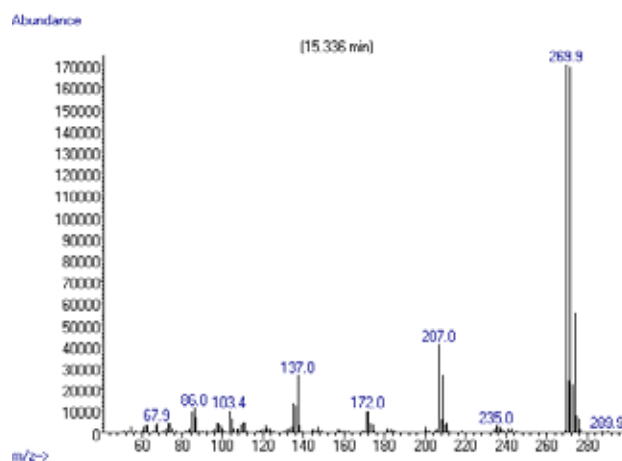


Figure 3: Mass spectrum of 2,4,8-Trichlorodibenzofuran (Cat.No 11789.12). Retention time 15.336



Triclosan and Derivatives:

Chiron No.	Structures	Description	Abbreviation	CAS number	Concentration	Solvent	Quantity
11802.12-50-NN		Triclosan	2,4,4'-Trichloro-2'-hydroxydiphenyl	3380-34-5	50 µg/mL	n-nonane	1 mL
11802.12-100-IO		Triclosan	2,4,4'-Trichloro-2'-hydroxydiphenyl	3380-34-5	100 µg/mL	isooctane	1 mL
11801.13-50-NN		Triclosan methyl ether	Triclosan-Methyl	4640-01-1	50 µg/mL	n-nonane	1 mL
Triclosan Impurities:							
2067.6-K-IP		3-Chlorophenol		108-43-0	1000 µg/mL	isopropanol	1 mL
2068.6-K-IP		4-Chlorophenol		106-48-9	1000 µg/mL	isopropanol	1 mL
2064.6-K-IP		2,4-Dichlorophenol		120-83-2	1000 µg/mL	isopropanol	1 mL
2038.12-50-NN		2,8-Dichlorodibenzofuran	PCDF 15 2,8-DiCDF	5409-83-6	50 µg/mL	n-nonane	1 mL
11789.12-50-NN		2,4,8-Trichlorodibenzofuran	PCDF 45 2,4,8-TriCDF	54589-71-8	50 µg/mL	n-nonane	1 mL
Internal Standards:							
11803.12-50-NN		Triclosan-d3 (2,4-dichlorophenoxy-d3)		1020719-98-5	50 µg/mL	n-nonane	1 mL
11804.13-50-NN		Triclosan methyl ether (methyl-d3)	Triclosan-Methyl-d3	1020720-00-6	50 µg/mL	n-nonane	1 mL
11808.6-K-IP		4-Chlorophenol-2,3,5,6-d4		285132-91-4	1000 µg/mL	isopropanol	1 mL
2422.6-K-IP		2,4-Dichlorophenol-3,5,6-d3		93951-74-7	1000 µg/mL	isopropanol	1 mL

Literature:

- (1) Thompson, A.; Griffin, P.; Stuetz, R.; and Cartmell, E. (2005). "The fate and Removal of Triclosan during Wastewater Treatment", *Water Environment Research* 77 (1), 63-7.
- (2) Bedoux, G.; Roig, B.; Thomas, O.; Dupont, V.; Le Bot, B. (2011). "Occurrence and toxicity of antimicrobial triclosan and by-products in the environment". *Environmental Science and Pollution Research* 19, (4), 1044-65.
- (3) "Triclosan Registration Review Preliminary Work Plan". *Environmental Protection Agency* 27 March 2013.
- (4) van den Berg, M.; van Birgelen A.; Birnbaum, L. Brouwer, B.; Carrier, G.; Dragan, Y.; Farland, W.;-Feeley, M.; Fyrst, P.; Galli, C.L.; Greig, J.; Hayashi, Y.; Kogevinas, M; Kurokawa, Y.; Larsen, J.C.; Liem, A.K.D.; Matsumura, F.; Mocarelli, P.; Moore, M.R., Newhook, R.C.; Peterson, R.E.; Poellinger, L. Portier, C. Rogan, W.J; Schrenk, D.; Sweeney, M.H.; Tohyama, C.; Tuomitso, J; Water; Zeilmaker, M. (2000) «Consultation on assessment of the health risk of dioxins; reevaluation of the tolerable daily intake (TDI): Executive Summary: Food Additives and Contaminants 17 (4); 223-40.
- (5) SCCP/1251/09. *European Commission Scientific Committee on Consumer Safety (SCCS): Opinion on Triclosan Antimicrobial Resistance. 22 June 2010.*

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