Environ. Chem. **2015**, *12*, 504–514
doi:10.1071/EN14210_AC

Supplementary material

Isotopic composition of polyhalomethanes from marine macrophytes – systematic effects of the halogen substituents on isotopic composition

Enno Bahlmann,[A,B,C] *Christian Stolle,*[B] *Ingo Weinberg,*[B] *Richard Seifert,*[A] *Detlef E. Schulz-Bull*[B] *and Walter Michaelis*[A]

[A]Department of Geosciences, University of Hamburg, Bundesstraße 55, D-20146 Hamburg, Germany.

[B]Leibniz Institute for Baltic Sea Research Warnemünde (IOW), Seestraße 15, D-18119 Rostock, Germany.

[C]Corresponding author. Email: enno.bahlmann@zmaw.de

Environ. Chem. **2015**, 12, 504–514
doi:10.1071/EN14210_AC

Table S1. Polyhalomethane (PHM) production rates (pmol g^{-1} FW h^{-1}) of *Fucus vesiculosus* and *F. serratus* during 24-h incubations (at Institute of Baltic Seas Research, IOW)

	F. vesiculosus			*Fucus serratus*			*Fucus vesiculosus*			*Fucus serratus*			
	Light, H_2O_2			Light, H_2O_2			Light			Light			
CH_3I	0.058	0.079	0.071	0.002	0.004	0.020			0.030				
CH_2BrCl	0.078	0.099	0.060	0.113	0.061	0.169							
$CHCl_3$	0.130	0.010	0.056	0.003	0.022	0.016						0.011	
CH_2Br_2	2.203	1.898	0.685		1.460	4.580	0.008	0.393	0.056	0.009	0.030	0.041	0.034
$CHBrCl_2$	0.055	0.040	0.022	0.057	0.006	0.092							
CH_2ClI	0.022	0.010	0.015		0.025	0.033							
$CHBr_2Cl$	0.082		0.016		0.073	0.234							
$CHBr_3$	4.318	13.480	0.801	10.164	23.286	9.850	0.003	0.406	0.090	0.040	0.112	0.114	0.013
CH_2I_2	0.019	0.037	0.039	0.006	0.044	0.026						0.013	

Table S2. Isotopic composition of polyhalomethanes (PHMs) (‰) from *Fucus vesiculosus* and *F. serratus* during 24-h incubations (at Institute of Baltic Seas Research, IOW)

	F. vesiculosus			*Fucus serratus*			*Fucus vesiculosus*			*Fucus serratus*			
	Light, H_2O_2			Light, H_2O_2			light			light			
CH_3I	–50.9	–45.6	–51.6	–41.7	–34.1	–40.4			–28			–31.6	
CH_2BrCl	–30.3	–31.4	–28.6	–29.5	–31.5	–29.5							
$CHCl_3$	–44	–38.1	–44.4	–36.5	–37.2	–35.3						–28.5	
CH_2Br_2	–31.3	–29.1	–32.4		–31	–31.1	–19.1	–18	–20.3	–19.4	–19.3	–17.9	–20
$CHBrCl_2$	–41.2	–41.7	–37.2	–35.6	–37.6	–40.5							
CH_2ClI	–11.3	–11.5	–11.7		–10.1	–11.7							
$CHBr_2Cl$	–35.3		–35.5		–31.5	–32.1			–28.3				
$CHBr_3$	–28	–22.9	–27.6	–23.8	–28.3	–27	–16.9	–11.2	–14.7	–18.5	–19.7	–14.7	–14.8
CH_2I_2	–24.6	–23.5	–21.5	–20.1	–22.7	–22.7						–21.5	

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Table S3. Polyhalomethane (PHM) production rates (pmol g^{-1} FW h^{-1}) from *Laminaria digitata* and *Fucus vesiculosus* incubations (at Institute of Biogeochemistry and Marine Chemistry, IFBM)

LW1, light and water at the beginning of the experiment; NLW, no light, water; LW2, light and water 16 h after the beginning of the experiment; LNW, light, no water; NLNW, no light, no water. Incubations with *L. digitata* were performed in two independent experiments with two different specimens (*L. digitata* 1 and 2)

	L. digitata 1															*L. digitata* 2			*F. vesiculosus*		
	LW1	LW1	LW1	LW1	LW1	DW	DW	LW2	LW2	LW2	LW2	LNW	LNW	NLNW	NLNW	LNW	LNW	LNW	LNW	LNW	LNW
CH_2Cl_2	0.8	0.4	0.4	0.4	0.3			0.2		0.3	0.1	0.1				0.4	0.4	0.3	0.3	0.2	
CH_2BrCl	2.6	3.1	4.0	2.7	3.4		1.0	0.7		0.4	1.6		0.3	0.2		5.6	5.3	5.3			
CH_2Br_2	68	81	92		90		36	8.5	6.9	19	24	15	10	7.2	4.2	152	109	70	0.7	1.5	0.2
CH_2ClI	17	35	51	51	55		6.2				2.2	1.0	0.6	0.6	0.2	7.2	7.3	4.9		0.2	
CH_2BrI	64	90	113	94	93		30	5.2		9.7	12	14	5.5	7.2	4.3	147	5.4	64			
CH_2I_2	355	527	649	356	376	4.4	104	6.1	10	17.0	27	51	11	20	12	280		172	2.4	12	1.3
$CHBrCl_2$	0.7	0.7	0.6	0.6						0.3	0.3	0.2				1.9	5.4	0.9			
$CHBr_2Cl$	15	16	17		13		5.4	7.2		3.9	5.0	3.7		2.0	0.8	33.7		36.1			
$CHBr_3$	232	278	346	261	356	12	156	29		76	104	58	9.5	29	14	590	398	338	10		3.5
$CHCl_2I$	1.9	2.4															1.1				
$CHBr_2I$		20	25	4.5	11.2									0.3		20		20			
$CHBrI_2$	1.8	1.6																			

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Table S4. Isotopic composition of polyhalomethanes (PHMs) (‰) from *Laminaria digitata* and *Fucus vesiculosus* incubations (at Institute of Biogeochemistry and Marine Chemistry, IFBM)

LW1, light and water at the beginning of the experiment; NLW, no light, water; LW2, light and water 16 h after the beginning of the experiment; LNW, light no water; NLNW, no light, no water. Incubations with *L. digitata* were performed in two independent experiments with two different specimen (*L. digitata* 1 and 2)

	L. digitata 1															*L. digitata* 2			*F. vesiculosus*		
	LW1	LW1	LW1	LW1	LW1	DW	DW	LW2	LW2	LW2	LW2	LNW	LNW	NLNW	NLNW	LNW	LNW	LNW	LNW	LNW	LNW
CH_2Cl_2		–39.7	–39.4		–43.2							–35.9				–42.4	–42.1	–41.0	–32.0	–37.8	
CH_2BrCl	–31.2	–31.0	–33.3	–31.9	–28.6		–32.7	–46.9			–31.1		–29.7			–44.8	–42.5	–38.2			
CH_2Br_2	–29.0	–28.0	–31.2		–27.4		–30.0	–31.5		–30.5	–29.4	–23.8	–25.8	–28.1	–30.6	–36.1	–35.7	–34.7	–17.7	–23.9	–8.7
CH_2ClI	–40.5	–40.7	–40.4	–33.2	–30.7		–30.3				–19.1	–23.4	–28.1	–33.5	–17.7	–44.0	–49.9	–45.4		–10.1	
CH_2BrI	–31.3	–28.2	–28.9	–26.2	–19.6		–23.0	–24.5		–20.7	–19.2	–21.7	–22.0	–23.2	–21.9	–37.9		–35.1			
CH_2I_2	–36.2	–32.6	–32.4	–26.5	–22.8	–12.9	–12.2	–7.9	–37.0	–11.0	–6.1	–9.6	–4.9	–8.6	–14.5	–22.7		–23.0	–17.3	–22.8	–16.0
$CHBrCl_2$	–38.1	–34.2		–29.4						–35.1	–34.5	–28.6				–46.5	–42.5	–28.2			
$CHBr_2Cl$	–28.9	–31.8	–33.4		–34.3		–34.0	–30.6		–30.8	–30.9	–32.0	n/a	–29.8	–33.1	–42.5		–37.9			
$CHBr_3$	–30.5	–29.7	–30.6	–26.9	–27.3	–24.6	–29.4	–32.2		–29.3	–27.5	–23.9	–28.4	–26.8	–33.0	–37.8	–35.8	–34.0	–21.3		–24.9
$CHCl_2I$	–27.0	–33.5															–38.9				
$CHBr_2I$		–10.7	–13.0	5.8	–5.9									3.4		–18.5		–24.2			
$CHBrI_2$	3.8	10.1																			

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Table S5. $CHBr_3$ production rates and isotopic composition from the *Zostera noltii* incubations

Fresh weight (FW) of *Z. noltii* was 33.9 g

	Experimental conditions	Production (pmol g^{-1} FW)	$\delta^{13}C$ (‰)
Z. noltii 1	Light, 2 h	3.6	–7.5
Z. noltii 2	Light, 2 h	–	
Z. noltii 3	Dark 14 h	0.9	–11.0
Z. noltii 4	Light, 2 h	5.3	–7.6
Z. noltii 5	Light, 2 h	5.5	–2.7
Z. noltii 6	Light, 2 h	4.5	–4.1
Z. noltii 7	Dark 14 h	0.8	–9.2
Z. noltii 8	Light, 2 h	5.9	–8.7
Z. noltii 9	Light, 2 h	3.8	–4.1
Z. noltii 10	Light, 2 h	–	
Z. noltii 11	Dark 16 h	0.5	–7.7
		(pmol L^{-1})	
Seawater 1	Light 3 h	20.9	–2.7
Seawater 2	Dark 16 h	3.3	–0.6
Seawater 4	Light 2 h	17.8	0.7
Seawater 5	Dark 16 h	1.8	1.8