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Supporting Information

Investigating the presence and persistence of volatile methylsiloxanes in Arctic sediments

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Table S1: Chemical names and identifiers for the volatile methylsiloxanes used in this study

Preferred chemical name	IUPAC name	Abbreviation	CAS number	InChIKey
Decamethyltetrasiloxane	Decamethyltetrasiloxane	L_4	141-62-8	YFCGDEUVHLPRCZ-UHFFFAOYSA-N
Dodecamethylpentasiloxane	Dodecamethylpentasiloxane	L_5	141-63-9	FBZANXDWQAVSTQ-UHFFFAOYSA-N
Tetradecamethylhexasiloxane	Tetradecamethylhexasiloxane	L_6	107-52-8	ADANNTOYRVPQLJ-UHFFFAOYSA-N
Octamethylcyclotetrasiloxane	2,2,4,4,6,6,8,8-Octamethyl-1,3,5,7,2,4,6,8-tetroxatetrasilocane	D_4	556-67-2	HMMGMWAXVFQUOA-UHFFFAOYSA-N
Decamethylcyclopentasiloxane	2,2,4,4,6,6,8,8,10,10-Decamethyl-1,3,5,7,9,2,4,6,8,10-pentoxapentasilecane	D_5	541-02-6	XMSXQFUHVRWGNA-UHFFFAOYSA-N
Dodecamethylcyclohexasiloxane	Dodecamethylcyclohexasiloxane	D_6	540-97-6	IUMSDRXLFWAGNT-UHFFFAOYSA-N

Table S2: Sampling locations with coordinates for each station and sampling dates for each sample.

Location	sample name	degrees N	degrees E	Sampling date
Svalbard Sediment	A1	78.24193	15.54158	Aug 15, 2016
	A2	78.24443	15.54904	Aug 15, 2016
	A3	78.24905	15.56556	Aug 15, 2016
	A4	78.14502	15.33502	Aug 15, 2016
	A5	78.24522	15.64872	Aug 15, 2016
Svalbard Wastewater	W1	Longyearbyen wastewater facility		Aug 20, 2016
	W2			Aug 20, 2016
	W3			Aug 20, 2016
	W4			Aug 20, 2016
	W5			Aug 20, 2016
	W6			Aug 20, 2016
		degrees N	degrees W	
Canada Sediment	C1	71.04770	133.38200	Aug 22, 2014
	C2	68.58234	105.28276	Aug 12, 2014
	C3	71.24558	157.28891	Sep 10, 2014
	C4	77.26476	76.22435	Oct 10, 2015
	C5	68.58234	105.28276	Aug 12, 2014
	C6	69.10269	100.41636	Aug 11, 2014
	C7	70.10000	133.33000	Aug 23, 2014
	C8	75.03680	167.08300	Sep 16, 2014
	C9	74.08370	108.49920	Sep 7, 2014
	C10	71.04770	133.38200	Aug 22, 2014
	C11	70.45862	72.15591	Oct 1, 2014
	C12	70.45862	72.15591	Oct 1, 2014
	C13	71.19314	70.38975	Oct 16, 2015
	C14	71.19314	70.38975	Oct 16, 2015
		degrees N	degrees E	
Greenland Sediment	G1	64.17662	-51.69445	Aug 23, 2016
	G2	64.17176	-51.68801	Aug 23, 2016
	G3	64.16585	-51.69204	Aug 23, 2016
	G4	64.15747	-51.70320	Aug 23, 2016
	G5	64.16309	-51.72380	Aug 23, 2016
	G6	64.16600	-51.72208	Aug 23, 2016
	G7	64.16845	-51.72037	Aug 23, 2016
	G8	64.16847	-51.72037	Aug 23, 2016
	G9	64.17311	-51.71213	Aug 23, 2016
	G10	64.14086	-51.61943	Aug 23, 2016

Table S3: Field blank concentrations (ng/g) for all three sampling locations corrected for the concentrations measured in the extraction blanks.

Field blanks (ng/g)	Location	L_4	L_5	L_6	D_4	D_5	D_6
Ammonium sulfate	Adventfjorden	0.014	0.018	0.0020	0.11	0.081	0.090
	Canada	0.0050	0	0	0.089	0.027	0.041
	Greenland	0.010	0.0010	0	0.12	0.087	0.092
	Average	0.010	0.0060	0.0010	0.11	0.065	0.074
	STD	0.0050	0.010	0.0010	0.016	0.033	0.029
Sand	Adventfjorden	0.034	0.0020	0.0010	0.20	0.041	0.075
	Canada	0.0010	0	0.0030	0.12	0.14	0.10
	Greenland	0.020	0	0	0.31	0.083	0.041
	Average	0.018	0.0010	0.0010	0.21	0.088	0.073
	STD	0.017	0.0010	0.0020	0.095	0.050	0.031
Sediment	Adventfjorden	0.035	0.010	0.0010	0.059	0.053	0.083
	Canada	0.039	0.013	0	0.14	0.074	0.046
	Greenland	0.030	0.0080	0	0.23	0.13	0.052
	Average	0.034	0.011	0	0.142	0.087	0.060
	STD	0.0050	0.0020	0	0.085	0.042	0.020

Table S4: Extraction blank concentrations in pg/μL of solvent extract.

Extraction blanks (pg/μL)	L_4	L_5	L_6	D_4	D_5	D_6
EB1	0.000	0.000	0.000	4.483	1.236	0.000
EB2	1.059	0.314	0.000	1.290	2.568	1.476
EB3	0.000	0.000	0.000	0.000	0.033	2.519
Average	0.353	0.105	0.000	1.924	1.279	1.332
SD	0.611	0.181	0.000	2.308	1.268	1.266

Table S5: Average recoveries for the sediment and wastewater samples.

	Extraction Recoveries (%)					
Sediment Samples	L_4	L_5	L_6	D_4	D_5	D_6
Svalbard	90 ± 12	82 ± 14	60 ± 15	90 ± 12	82 ± 14	60 ± 15
Canada	91 ± 11	85 ± 9	64 ± 13	91 ± 11	85 ± 9	64 ± 13
Greenland	86 ± 19	75 ± 10	66 ± 10	86 ± 19	75 ± 10	66 ± 10
Wastewater Samples	-	-	-	82 ± 14	70 ± 19	66 ± 22

Table S6: Concentrations of VMS (ng/g wet weight) and total organic carbon (TOC, %) in sediments from Svalbard (Adventfjorden), Canada (Archipelago), Greenland (Nuuk Harbor). Concentrations below the limit of quantification are shown as <LOQ. For the purposes of descriptive statistics, the average and standard deviation were calculating after assigning a value of 0 to the samples that were below the LOQ. An explanation as to why this choice was made is presented in the Statistics section of the main manuscript.

		(ng/g) wet weight						
Location	Sample	L4	L5	L6	D4	D5	D6	TOC (%)
Svalbard	A1	0.068	<LOQ	<LOQ	0.56	0.47	<LOQ	1.3
	A2	<LOQ	<LOQ	0.027	<LOQ	0.72	0.21	1.6
	A3	<LOQ	<LOQ	0.0018	0.68	0.67	<LOQ	2.1
	A4	<LOQ	<LOQ	0.0024	<LOQ	<LOQ	<LOQ	2
	A5	<LOQ	<LOQ	0.0034	0.85	0.82	<LOQ	1.9
	Average	0.014	0	0.0087	0.42	0.54	0.042	1.78
	STD	0.030	0	0.012	0.39	0.32	0.094	0.33
Canada	C1	0.61	<LOQ	0.02	0.96	1.7	1	0.12
	C2	0.046	<LOQ	<LOQ	<LOQ	0.14	<LOQ	0.18
	C3	0.3	<LOQ	0.016	2.7	3.5	0.68	0.23
	C4	0.36	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	0.5
	C5	0.96	<LOQ	0.045	4.7	4	2.7	1.1
	C6	0.099	<LOQ	<LOQ	1.8	19	<LOQ	0.6
	C7	0.086	<LOQ	0.0026	1	1.2	0.18	1.2
	C8	0.075	<LOQ	0.0014	0.25	0.21	0.094	1.1
	C9	0.078	<LOQ	<LOQ	0.4	0.36	0.13	0.05
	C10	0.31	<LOQ	0.013	1.4	2.5	0.87	0.06
	C11	0.11	<LOQ	<LOQ	0.52	0.38	<LOQ	0.16
	C12	0.084	<LOQ	<LOQ	0.9	0.89	<LOQ	0.95
	C13	0.039	<LOQ	<LOQ	0.37	0.31	<LOQ	0.3
	C14	0.25	<LOQ	<LOQ	1.5	1.5	0.47	0.4
	Average	0.24	0	0.007	1.18	2.55	0.44	0.5
	STD	0.26	0	0.013	1.26	4.90	0.74	0.42
Greenland	G1	0.28	0.2	0.047	5.9	10	1.4	1
	G2	0.15	0.09	0.015	1.5	1.9	0.36	1.8
	G3	0.17	0.1	0.018	6.9	1.8	0.38	2
	G4	0.72	0.22	0.04	6.2	26	9.8	0.6
	G5	0.17	0.096	0.019	6	3.5	0.55	3
	G6	0.21	0.023	0.007	6.9	4.1	0.51	1.6
	G7	0.5	0.44	0.073	10	5.7	0.86	1.8
	G8	0.64	0.34	0.064	5.1	5.5	1	2.6
	G9	0.13	0.12	0.023	3.1	0.9	0.43	0.31
	G10	0.054	0.029	0.0073	1.5	2.8	0.59	0.1
	Average	0.30	0.17	0.031	5.31	6.22	1.59	1.48
	STD	0.23	0.14	0.024	2.64	7.43	2.90	0.96

Table S7: Average concentrations (ng/L) and standard deviations of cVMS in wastewater and from Svalbard (Adventfjorden).

	D_4	D_5	D_6
Average C (ng/L)	39.8	156	32.6
STD (n = 3)	11.8	83.1	14.1
Field blank (ng/L)	6.7	5.1	5,9
STD (n = 3)	2.3	1.0	0.4
LOQ (ng/L)	29.4	15.2	9.7

Table S8: Correlations between concentrations and TOC

		L_4	D_4	L_5	D_5	L_6	D_6
R^2	Svalbard	0.63	0.008	NA	0.17	0.28	0.13
	Canada	0.014	0.081	NA	0.0085	0.028	0.034
	Greenland	0.02	0.16	0.058	0.075	0.047	0.1
coefficient	Svalbard	-0.08	0.11	NA	-0.17	-0.01	-0.1
	Canada	0.21	0.84	NA	1.03	0.0051	0.32
	Greenland	0.03	1.1	0.034	-2.2	0.0053	-0.98
p-value	Svalbard	0.09	0.088	NA	0.79	0.65	0.55
	Canada	0.1	0.32	NA	0.76	0.57	0.53
	Greenland	0.7	0.26	0.5	0.44	0.55	0.37

Table S9: Statistics for samples from Canadian Archipelago. The samples were divided into two groups based on the median value for distance from the nearest settlement, distance from the nearest land and distance from nearest major river mouth. We calculated average values, standard deviations and p-values for the t-tests that were used to compare the various groups.

Location	Sample	L4	L5	L6	D4	D5	D6	TOC (%)	Distance from settlement (mi)	Distance from land (mi)	Distance from major river mouth (mi)
Canada	C1	0.61	0	0.02	0.96	1.7	1	0.12	129	97.7	123
	C2	0.046	0	0	0	0.14	0	0.18	34.2	0.5	112
	C3	0.3	0	0.016	2.7	3.5	0.68	0.23	11.7	7.6	688
	C4	0.36	0	0	0	0	0	0.5	82	30.7	688
	C5	0.96	0	0.045	4.7	4	2.7	1.1	35.8	0.5	710
	C6	0.099	0	0	1.8	19	0	0.6	115	0.1	710
	C7	0.086	0	0.0026	1	1.2	0.18	1.2	47	34.3	266
	C8	0.075	0	0.0014	0.25	0.21	0.094	1.1	332	322	516
	C9	0.078	0	0	0.4	0.36	0.13	0.05	226	48	806
	C10	0.31	0	0.013	1.4	2.5	0.87	0.06	109	101	171
	C11	0.11	0	0	0.52	0.38	0	0.16	83.4	0.01	100
	C12	0.084	0	0	0.9	0.89	0	0.95	83.4	0.01	50.5
	C13	0.039	0	0	0.37	0.31	0	0.3	64	9.3	779
	C14	0.25	0	0	1.5	1.5	0.47	0.4	64	9.3	451
Average for less than median distance from nearest settlement		0.348	0.000	0.016	2.100	2.210	0.890	0.678	32.175	-	-
STD for less than median distance from nearest settlement		0.423	0.000	0.021	2.061	1.841	1.240	0.548	14.790	-	-
Average for more than median distance from nearest settlement		0.202	0.000	0.003	0.810	2.685	0.256	0.424	128.780	-	-
STD for more than median distance from nearest settlement		0.181	0.000	0.007	0.601	5.788	0.387	0.368	85.655	-	-
Average for less than median distance from land		0.236	0.000	0.008	1.561	3.715	0.481	0.490	-	3.415	-
STD for less than median distance from land		0.307	0.000	0.016	1.539	6.349	0.935	0.361	-	4.439	-
Average for more than median distance from land		0.253	0.000	0.006	0.668	0.995	0.379	0.505	-	105.617	-
STD for more than median distance from land		0.216	0.000	0.008	0.534	0.981	0.437	0.527	-	110.385	-
Average for less than median distance from a major river mouth		0.207	0.000	0.005	0.807	1.060	0.334	0.310	-	-	471.000
STD for less than median distance from a major river mouth		0.206	0.000	0.008	0.546	0.873	0.446	0.304	-	-	288.799
Average for more than median distance from a major river mouth		0.280	0.000	0.009	1.550	4.039	0.541	0.683	-	-	410.500
STD for more than median distance from a major river mouth		0.322	0.000	0.017	1.684	6.791	0.980	0.459	-	-	313.144
T-test p-value for distance from settlement		0.516	-	0.571	0.425	0.466	0.512	0.601	-	-	-
T-test p-value for distance from land		0.452	-	0.415	0.081	0.135	0.395	0.477	-	-	-
T-test p-value for distance from a major river mouth		0.313	-	0.267	0.151	0.146	0.313	0.051	-	-	-

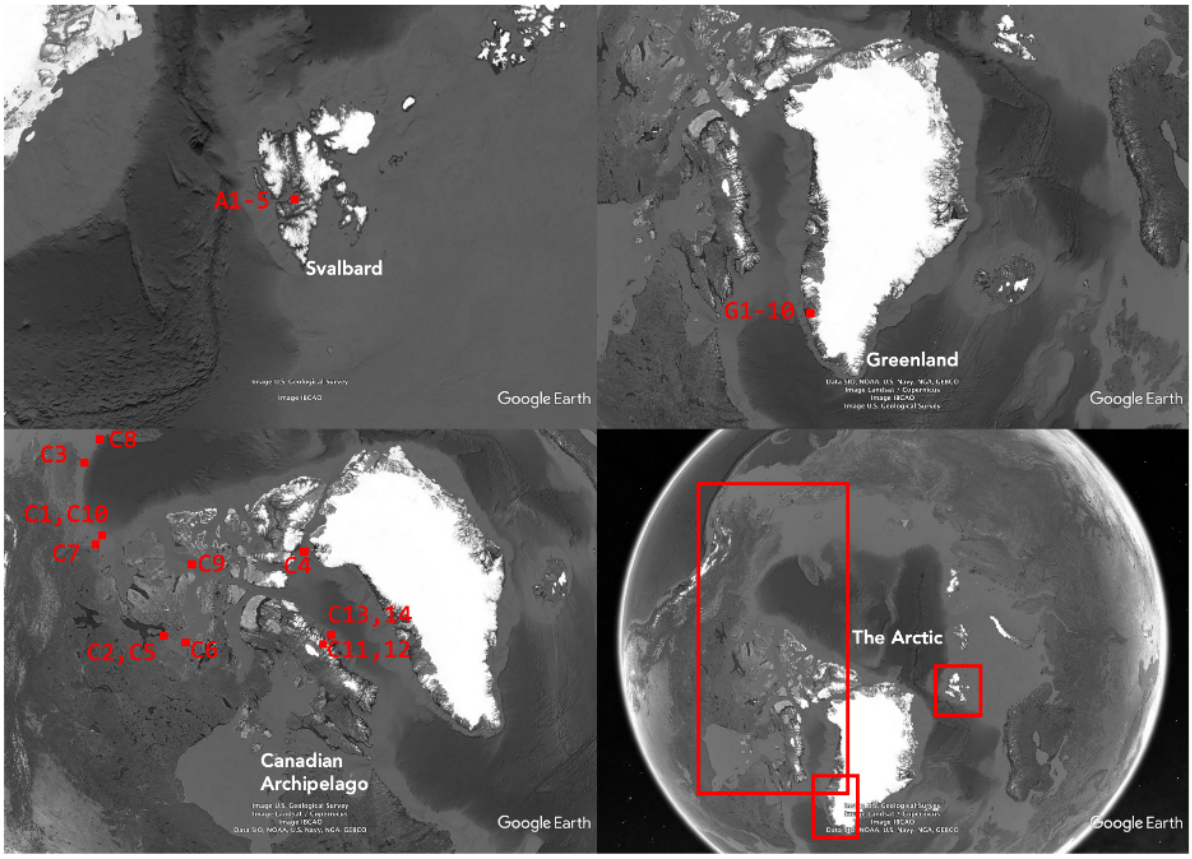

Figure S1: Geographical regions and sampling stations for the collection of sediment samples in Svalbard (Adventfjorden), Greenland (Nuuk Harbor) and Canada (Canadian Archipelago). The sampling regions and stations are shown in red.