

**Linear and Branched Perfluorooctane Sulfonate Isomer
Patterns in Herring Gull Eggs from Colonial Sites Across the
Laurentian Great Lakes**

Wouter A. Gebbink and Robert J. Letcher

National Wildlife Research Centre, Science and Technology Branch, Environment

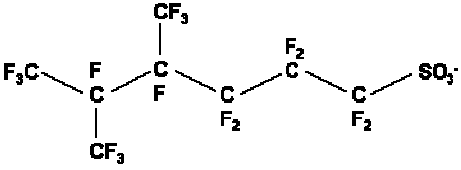
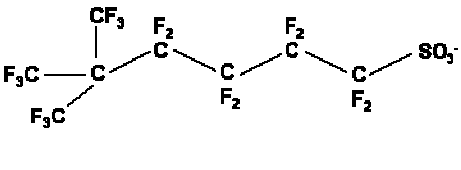
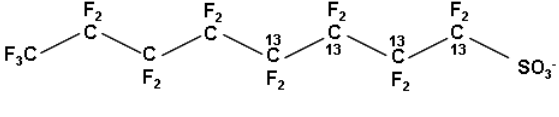
Canada, Carleton University, Ottawa, ON, K1A 0H3, Canada

Department of Chemistry, Carleton University, Ottawa, Ontario, K1S 5B6, Canada

SUPPORTING INFORMATION

Table S1. Chemical Names and Abbreviations and Two-Dimensional Chemical Structures of Linear and Branched, Geometric Perfluorooctane Sulfonate (PFOS) Isomers.

Chemical Name	Abbreviation	PFOS Isomer Chemical Structure
<i>n</i> -perfluoro-1-octanesulfonate	L-PFOS	
perfluoro-1-methyl-heptanesulfonate	P1MHpS	
perfluoro-2-methyl-heptanesulfonate	P2MHpS	
perfluoro-3-methyl-heptanesulfonate	P3MHpS	
perfluoro-4-methyl-heptanesulfonate	P4MHpS	
perfluoro-5-methyl-heptanesulfonate	P5MHpS	
perfluor-6-methyl-heptanesulfonate	P6MHpS	
perfluoro-3,5-dimethyl-hexanesulfonate	P35DMHxS	
perfluoro-4,4-dimethyl-hexanesulfonate	P44DMHxS	

perfluoro-4,5-dimethyl-hexanesulfonate	P45DMHxS	
perfluoro-5,5-dimethyl-hexanesulfonate	P55DMHxS	
<i>n</i> -perfluoro-1-[1,2,3,4- ¹³ C ₄]octanesulfonate	M-L-PFOS ^a	

^a Internal standard.

Table S2. Correlations between Concentrations (ng/g ww) of Individual Mono(trifluoromethyl) Perfluorooctane Sulfonate (PFOS) Isomers and Σ PFOS in Individual Herring Gull Eggs (n=13) from 15 Colonies in the Great Lakes Collected in 2007.

Colony# ^a	Location		PFOS Isomer ^b					
			P1MHpS	P2MHpS	P3MHpS	P4MHpS	P5MHpS	P6MHpS
1	Granite Is.	r	0.871	0.770	0.847	0.838	0.926	0.942
		p	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
2	Agawa Rocks	r	0.744	0.602	0.281	0.392	0.222	0.774
		p	0.001	0.02	0.31	0.15	0.43	0.0007
3	Big Sister Is.	r	0.639	0.779	0.631	0.778	0.813	0.804
		p	0.01	0.0006	0.01	0.0006	0.0002	0.0003
4	Gull Is.	r	0.364	0.337	0.376	0.487	0.612	0.435
		p	0.18	0.22	0.17	0.07	0.02	0.10
5	Channel-Shelter Is.	r	0.845	0.253	-0.368	-0.360	-0.330	-
		p	<0.0001	0.36	0.18	0.19	0.23	-
6	Double Is.	r	0.879	0.767	0.653	0.733	0.820	0.863
		p	<0.0001	0.0008	0.008	0.002	0.0002	<0.0001
7	Chantry Is.	r	0.945	0.843	0.670	0.384	0.766	0.947
		p	<0.0001	<0.0001	0.006	0.16	0.0009	<0.0001
8	Fighting Is.	r	0.919	0.962	0.857	0.855	0.853	0.919
		p	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001	<0.0001
9	Middle Is.	r	0.819	0.848	0.684	0.877	0.819	0.358
		p	0.0002	<0.0001	0.005	<0.0001	0.0002	0.19
10	Port Colborne	r	0.862	0.867	0.815	0.845	0.783	0.759
		p	<0.0001	<0.0001	0.0002	<0.0001	0.0006	0.001
11	Niagara River	r	0.924	0.950	0.796	0.798	0.743	0.895
		p	<0.0001	<0.0001	0.0004	0.0004	0.001	<0.0001
12	Hamilton Harbour	r	0.561	0.590	0.451	0.694	0.824	0.913
		p	0.03	0.02	0.09	0.004	0.0002	<0.0001
13	Toronto Harbour	r	0.856	0.908	0.828	0.834	0.738	0.899
		p	<0.0001	<0.0001	0.0002	0.0001	0.002	<0.0001
14	Snake Is.	r	0.718	0.711	0.633	0.673	0.747	0.908
		p	0.003	0.003	0.01	0.006	0.001	<0.0001
15	Strachan Is.	r	0.533	0.213	0.107	0.190	0.300	0.565
		p	0.04	0.45	0.70	0.50	0.28	0.03

^a See Figure 1 for exact location of the 15 colonies

^b See Table S1 for names, abbreviations and structures of the linear and branched PFOS isomers. See Figure S1 for a typical GC-MS(ECNI) mass chromatogram showing PFOS isomers in a typical herring gull egg sample

Figure S1. GC-MS(ECNI) mass chromatogram of linear and branched, geometric perfluorooctane sulfonate (PFOS) isomers in a representative herring gull egg from Strachan Island, Lake Ontario.

Figure S2. Plot of arithmetic mean PFOS concentration ($\pm$ SE ng/g ww) obtained by LC-MSMS analysis (I) and arithmetic mean Σ PFOS concentration ($\pm$ SE ng/g ww) obtained by the present GC-MS analysis of individual herring gull eggs (n=13) from 15 colonies in the Great Lakes.

Reference List

- 1 Gebbink, W. A.; Hebert, C. E.; Letcher, R. J. Perfluorinated carboxylates and sulfonates and precursor compounds in herring gull eggs from colonies spanning the Laurentian Great Lakes of North America. *Environ. Sci. Technol.* **2009**, 43, 7443-7449.

