Supporting Information

Occurrence of Atrazine and Related Compounds in the Sediments of Upper Great Lakes

Jiehong Guo, Zhuona Li, Prabha Ranasinghe, Solidea Bonina, Soheil Hosseini, Margaret B. Corcoran, Colin Smalley, Rajashankar Kaliappan, Yan Wu, Da Chen, Andy L. Sandy, Yawei Wang, Karl J. Rockne, Neil C. Sturchio, John P. Giesy, An Li*

* correspondence author email: anli@uic.edu

Summary of Contents

14 pages, 8 Tables, 5 Figures

Table of Content

Table S1. Physicochemical properties of target herbicides

Figure S1. Sampling sites

Table S2. Sampling related information

Table S3-a. Multiple reaction mechanism transition in GCQQQ

Table S3-b. Transitions and some parameters in LC/MS/MS

Figure S2-a. Partial GC/EIQQQ-MS chromatograms of (A) top sediment (2-3 cm) extract from sampling site M018; (B) and (C) standard mixtures of simazine, atrazine and alachlor

Figure S2-b. LC/MS/MS chromatograms of (A) top sediment (2-3 cm) from sampling site M018; and (B) standard mixture

Table S4. Summary of measured core surface concentrations, and estimated inventory and recent flux of atrazine and related compounds in the sediments of Lakes Michigan, Superior and Huron

Table S5. Concentrations of atrazine and related compounds in natural sediments

Figure S3. Spatial distribution of atrazine, DEA and alachlor concentrations in Ponar grab samples from Lake Superior and Lake Huron

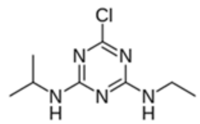
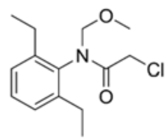
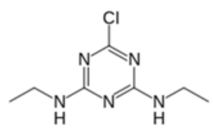
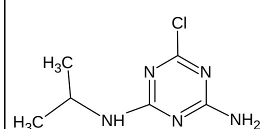
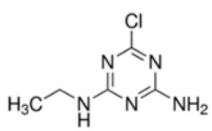
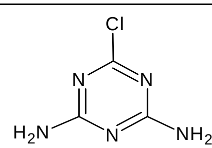
Figure S4. Comparison of median concentrations in Ponar grab samples among eight arbitrarily divided areas.

Table S6. Fisher's exact test for area comparison of chemical concentrations in Ponar grab samples.

Table S7. Pearson correlations among concentrations of target chemicals (natural log transformed) measured in PG sediments of Lakes Michigan, Superior and Huron for the concentrations above detection limits

Table S8. Summary of accumulation rate constant (k), doubling time and the first order kinetic regression statistics (r and *p*) at each coring site of Lakes Michigan, Superior and Huron

Table S1. Physicochemical properties of target herbicides [1, 2]

Chemicals	MW	structure	formula	water solubility (mg/L) at 25°C	vapor pressure (Pa) at 20°C	Henry's law constant ($Pa.m^3/mol$)	Log K_{ow}	Log K_{oc}
atrazine [a]	215.68		$C_8H_{14}ClN_5$	33.8 [3]	4.00E-05	2.88E-04	2.75	2.35 [2]
alachlor [a]	269.77		$C_{14}H_{20}ClNO_2$	240	2.88E-03	2.20E-03	2.8	2.23
simazine [a]	201.67		$C_7H_{12}ClN_5$	5	8.50E-06	3.43E-04	2.18	2.11
desethyl atrazine (DEA) [b]	187.63		$C_6H_{10}ClN_5$	3,200 [3]	1.51E-01	1.55E-04	1.51 [4]	1.935, 1.9 [5]
desisopropyl atrazine (DIA) [b]	173.6		$C_5H_8ClN_5$	670 [3]	2.81E-02	7.83E-04	1.15 [4]	1.746, 2.11 [5]
desethyldesisopropyl atrazine (DDA) [b]	145.55		$C_3H_4ClN_5$	42,020	3.27E-02	1.13E-04	0.32	1.318

[a] Unless specified, the data were obtained from Ref. [1]; [b] Unless specified, the data were obtained from U.S. EPA EPI SUITE or Ref. [2];

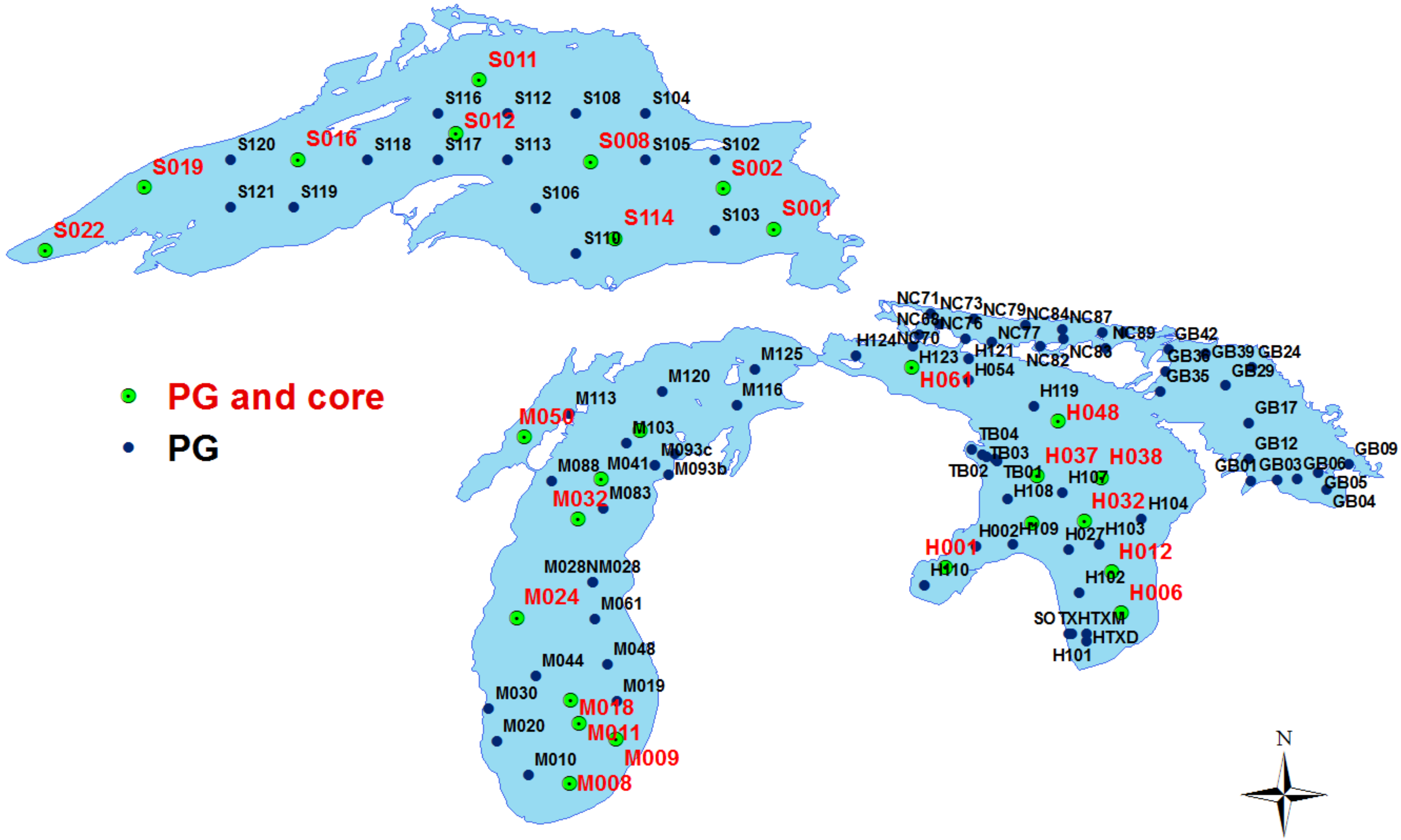


Figure S1. Sampling sites (PG: Ponar grab; labels for the sites are not all shown).

Table S2. Sampling related information

Site[a]	Date	Latitude	Longitude	Depth (m)	MSR[b]	Focus Factor
			Lake Michigan			
M008	9/20/2010	41.9842	-87.0142	64	*0.021*	0.49
M009	9/20/2010	42.3850	-86.5915	60	0.065	2.2
M010	9/17/2010	42.0662	-87.3792	50		
M011	9/20/2010	42.5283	-86.9220	160	0.041	2.99
M018	9/20/2010	42.7338	-86.9995	161	0.018	1.52
M019	9/20/2010	42.7335	-86.5833	90		
M020	9/17/2010	42.3665	-87.6672	45		
M024	9/17/2010	43.4830	-87.4882	146	0.019	1.98
M028	9/19/2010	43.8003	-86.7998	133		
M028N[c]	5/23/2011	43.7998	-86.7997	133		
M030	9/17/2010	42.6600	-87.7382	18		
M032	9/18/2010	44.3715	-86.9333	250	0.018	2.09
M041	9/19/2010	44.7367	-86.7215	265		
M041N[c]	5/24/2011	44.7375	-86.7221	266	0.022	2.11
M044	9/17/2010	42.9528	-87.3155	90		
M047	9/18/2010	45.1783	-86.3745	195	0.031	2.64
M048	9/19/2010	43.0585	-86.6630	104		
M050	9/18/2010	45.1165	-87.4165	32	0.043 (1–7)[d] 0.020 (8–19)[d]	2.85
M061	9/19/2010	43.4742	-86.7847	133		
M083	9/19/2010	44.4737	-86.7060	263		
M088	9/18/2010	44.7187	-87.1740	92		
M093a	9/19/2010	44.9622	-86.0552	97		
M093b	9/19/2010	44.7712	-86.1168	58		
M093c	9/19/2010	44.8562	-86.243	126		
M103	9/19/2010	45.0623	-86.4918	201		
M113	9/18/2010	45.3267	-87.009	36		
M116	5/24/2011	45.4014	-85.4997	36		
M120	9/18/2010	45.5288	-86.1708	136		
M125	5/24/2011	45.7228	-85.3314	16		
			Lake Superior			
S001	5/25/2011	46.9930	-85.1612	98	N/A[e]	0.09
S002	5/25/2011	47.3603	-85.6208	158	*0.0068*	0.82
S008	5/25/2011	47.6058	-86.8177	309	*0.0067*	0.76
S011	5/28/2011	48.3438	-87.8250	236	0.015	2.45
S012	5/28/2011	47.8553	-88.0418	245	0.0098	1.84
S016	5/27/2011	47.6212	-89.4633	185	0.0074	1.01
S019	5/26/2011	47.3703	-90.8535	193	*0.0088*	0.62

S022	5/27/2011	46.8002	-91.7508	56	*0.018* (1–7)[d]	0.6
					0.025 (8–25)[d]	
S102	5/25/2011	47.6173	-85.6973	95		
S103	5/29/2011	46.9838	-85.6972	169		
S104	5/26/2011	48.0382	-86.3217	194		
S105	5/25/2011	47.6177	-86.3217	83		
S106	5/28/2011	47.1807	-87.3183	225		
S108	5/26/2011	48.0392	-86.9493	233		
S110	5/28/2011	46.7735	-86.9495	142		
S112	5/28/2011	48.0393	-87.5733	222		
S113	5/28/2011	47.6177	-87.5730	176		
S114	5/28/2011	46.9095	-86.5980	409	N/A[e]	0.63
S116	5/28/2011	48.0392	-88.2007	261		
S117	5/28/2011	47.6175	-88.2007	277		
S118	5/27/2011	47.6175	-88.8420	194		
S119	5/27/2011	47.1955	-89.5048	202		
S120	5/26/2011	47.6185	-90.0712	183		
S121	5/27/2011	47.1955	-90.0727	150		

Lake Huron

GB01	10/6/2012	44.7178	-80.8564	93		
GB03	10/6/2012	44.7253	-80.6170	34		
GB04	10/6/2012	44.6457	-80.1673	59		
GB05	10/6/2012	44.7969	-80.2431	60		
GB06	10/6/2012	44.7382	-80.4360	88		
GB09	10/6/2012	44.8716	-79.9675	29.9		
GB12	10/6/2012	44.9202	-80.8748	91		
GB17	10/6/2012	45.2449	-80.8742	80		
GB24	10/6/2012	45.7457	-80.8394	31		
GB29	10/5/2012	45.5836	-81.0830	44		
GB35	10/5/2012	45.5257	-81.6705	37		
GB36	10/5/2012	45.7082	-81.6201	54		
GB39	10/5/2012	45.8729	-81.2584	26.9		
GB42	10/5/2012	45.9125	-81.5954	26		
H001	9/16/2012	43.9374	-83.6142	12.7	0.16	>3.24
H002	9/16/2012	44.1249	-83.3324	18.8		
H006	9/16/2012	43.5265	-82.0185	62	0.032 (1–10)[d]	2.17
					0.0083 (11–25)[d]	
H012	9/16/2012	43.9007	-82.1130	99	0.057	3.49
H027	9/16/2012	44.0999	-82.5025	65		
H032	9/16/2012	44.3542	-82.3596	94	0.044	3.16
H037	9/17/2012	44.7619	-82.7836	76	N/A[e]	0.87
H038	9/17/2012	44.7507	-82.2024	166	*0.0087*	0.89
H048	9/17/2012	45.2614	-82.5912	183	0.017	1.6
H054	9/18/2012	45.6338	-83.4028	142		
H061	9/18/2012	45.7498	-83.9164	122	*0.0063*	0.6

H095	9/16/2012	44.3328	-82.8326	70	0.014	1.13
H101	9/15/2012	43.2690	-82.3349	31		
H102	9/16/2012	43.7059	-82.4039	53		
H103	9/16/2012	44.1449	-82.2209	99		
H104	9/16/2012	44.3720	-81.8380	132		
H107	9/17/2012	44.6154	-82.5541	66		
H108	9/17/2012	44.5574	-83.0502	55		
H109	9/16/2012	44.1502	-83.0000	35		
H110	9/17/2012	43.7723	-83.8037	6.72		
H118	9/17/2012	44.9168	-83.1660	46		
H119	9/17/2012	45.3977	-82.8107	135		
H121	10/4/2012	45.8189	-83.4039	45		
H123	9/18/2012	45.9365	-83.9059	30		
H124	9/18/2012	45.8512	-84.4216	57		
NC68	10/4/2012	46.0413	-83.8536	16.4		
NC70	10/4/2012	46.1365	-83.6720	21.7		
NC71	10/4/2012	46.2335	-83.7462	36		
NC73	10/5/2012	46.1869	-83.3552	19.2		
NC76	10/5/2012	46.0003	-83.4329	60		
NC77	10/5/2012	45.9704	-83.1977	80		
NC79	10/5/2012	46.1230	-82.8867	26.2		
NC82	10/5/2012	45.9369	-82.7588	28.4		
NC83	10/5/2012	46.0000	-82.5497	31		
NC84	10/5/2012	46.0917	-82.5564	36		
NC87	10/5/2012	46.0611	-82.1971	41		
NC88	10/5/2012	46.0553	-81.9998	37		
NC89	10/5/2012	45.9165	-82.1617	39		
TB01	10/7/2012	44.8996	-83.1496	50		
TB02	10/7/2012	44.9387	-83.2405	31		
TB03	10/7/2012	44.9552	-83.2770	18.6		
TB04	10/7/2012	44.9997	-83.3742	10.3		
SOTXD	9/15/2012	43.3399	-82.3335	37		
SOTXM	9/15/2012	43.3398	-82.4668	19.6		
SOTXS	9/15/2012	43.3397	-82.4991	12.1		

[a] Coring sites are in bold font
[b] Mass sedimentation rate in g/cm^2-y. Those in italics should be read with caution due to low Pb-210 abundance thus higher uncertainty.
[c] Sampled in 2011.
[d] The numbers in the parentheses are core depth in cm
[e] Not available

Table S3-a. Multiple reaction mechanism transition in GC/QQQMS

Chemicals	Precursor	Quantification		Qualification	
		Ion	CE[a]	Ion	CE[a]
atrazine	214.9	200	7	173	5
simazine	200.9	173	5	186	5
alachlor	237	160	9	188	7
TBP-d27	231.1	103	11	167	1
PCB47L	303.8	234	31	269	13
Flu-d10	175.9	174	27	172	43
DDA	144.9	110	9	68	25
DIA	144.9	110	9	68	25
DEA	144.9	110	9	68	25

[a] collision energy

Table S3-b. Transitions and some parameters in LC/MS/MS

<table>
<tr><th></th><th>Q1[a] (m/z)</th><th>Q3[b] (m/z)</th><th>DP[c] (V)</th><th>EP[d] (V)</th><th>CEP[e] (V)</th><th>CE[f] (V)</th><th>CXP[g] (V)</th><th>CUR[h]</th><th>TEM[i] (°C)</th><th>IS[j] (V)</th><th>GS1[k]</th><th>GS2[l]</th></tr>
<tr><td rowspan="2">Atrazine</td><td>216.1</td><td>174.1</td><td>50</td><td>10</td><td>30</td><td>20</td><td>2</td><td rowspan="8">20</td><td rowspan="8">600</td><td rowspan="8">3000</td><td rowspan="8">80</td><td rowspan="8">90</td></tr>
<tr><td>216.1</td><td>104.1</td><td>50</td><td>10</td><td>30</td><td>50</td><td>2</td></tr>
<tr><td rowspan="2">DEA</td><td>188.1</td><td>146.2</td><td>50</td><td>10</td><td>30</td><td>40</td><td>2</td></tr>
<tr><td>188.1</td><td>104.1</td><td>50</td><td>10</td><td>30</td><td>40</td><td>2</td></tr>
<tr><td rowspan="2">DIA</td><td>174.1</td><td>104.1</td><td>45</td><td>10</td><td>25</td><td>40</td><td>2</td></tr>
<tr><td>174.1</td><td>68.1</td><td>45</td><td>8</td><td>25</td><td>50</td><td>8</td></tr>
<tr><td rowspan="2">DDA</td><td>146.1</td><td>79.1</td><td>55</td><td>10</td><td>25</td><td>40</td><td>2</td></tr>
<tr><td>146.1</td><td>68.0</td><td>55</td><td>10</td><td>30</td><td>50</td><td>2</td></tr>
</table>

[a] Precursor Ion; [b] Product Ion; [c] Declustering Potential; [d] Entrance Potential; [e] Collision Cell Entrance Potential; [f] Collision Energy; [g] Collision Cell Exit Potential; [h] Curtain Gas; [i] Temperature; [j] Ion Spray Voltage; [k] Ion Source Gas 1; [l] Ion Source Gas 2.

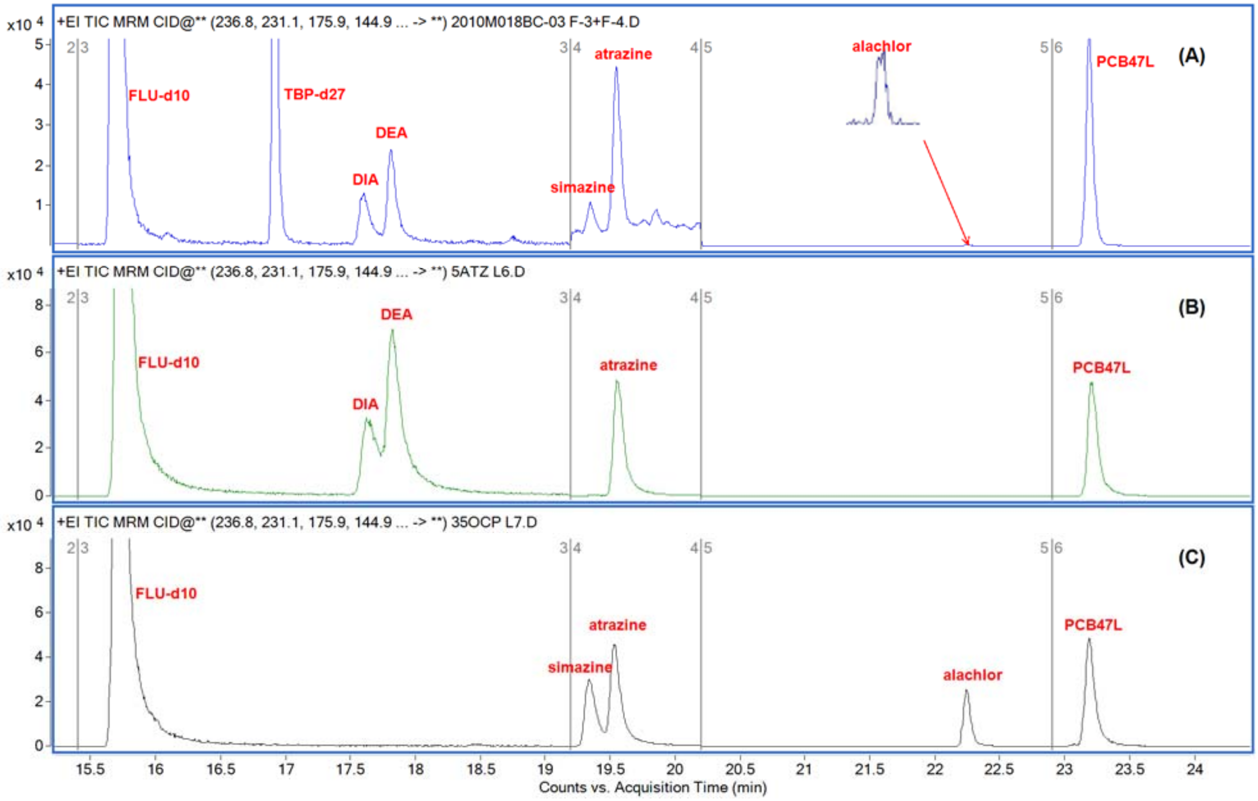


Figure S2-a. Partial GC/EIQQQ-MS chromatograms of (A) sample extracts for sediment core M018 segment (2-3 cm), and (B) standard mixture of targeted atrazine, DIA, and DEA, and (C) standard mixture of simazine, atrazine and alachlor.

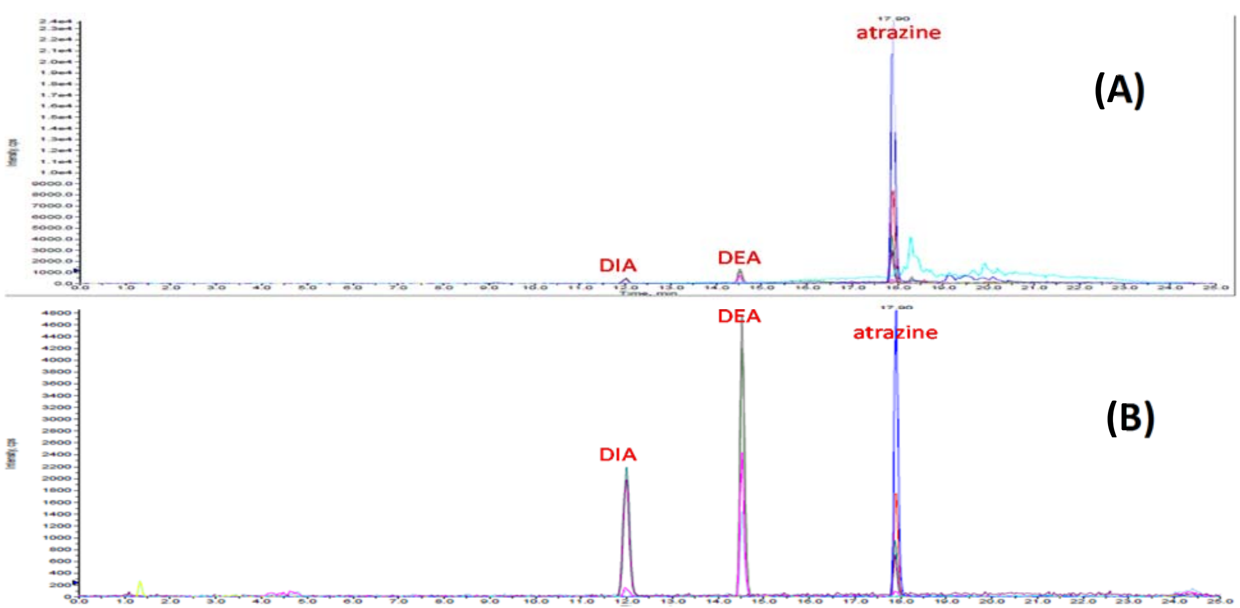


Figure S2-b. LC/MS/MS chromatograms of (A) sample extracts for sediment core M018 segment (2-3 cm), and (B) standard mixture of atrazine, DIA and DEA

Table S4. Summary of measured core surface concentrations, estimated inventory and recent flux of atrazine and related compounds in the sediments of Lakes Michigan, Superior and Huron

Core	Surface (0-1 cm) Concentration (ng/g dw [a])				Inventory (ng/cm^2)				Recent net deposition flux (ng/m^2-yr)			
	atrazine	DEA	simazine	alachlor	atrazine	DEA	simazine	alachlor	atrazine	DEA	simazine	alachlor
M008	4.02		1.04	0.17	5.15		4.85	0.32	1718		444	73
M009	4.14		1.26	0.33	5.85		1.32	0.66	1228		373	98
M011	5.87	2.77	1.54	0.18	6.36	3.92	2.37	0.45	798	376	209	25
M018	6.18	2.60	1.64	0.19	7.46	3.84	1.87	0.19	744	314	198	23
M024	5.43		1.90	0.30	8.90		3.35	0.32	527		184	29
M032	4.10	1.25	1.91	0.19	3.76	0.94	1.48	0.21	362	110	168	17
M041	5.40	2.31	1.39	0.10	7.07	4.34	0.98	0.11	566	242	145	10
M047	4.94		1.30	0.11	5.67		1.15	0.20	582		154	13
M050	2.53			0.06	1.61		0.39	0.16	382			9
S001	0.10	0.57			0.12	0.63						
S002	1.31			0.12	0.51	0.40		0.04	109			10
S008	1.55	1.21		0.06	0.68	1.29		0.02	138	107		5
S011	1.66	1.20		0.06	0.95	1.54		0.03	103	75		4
S012	0.82	0.90		0.06	0.53	1.06		0.02	43	48		3
S016	0.90	0.89			0.43	0.71			66	65		
S019	1.48	1.51		0.01	0.75	0.90		0.07	210	214		1
S022	1.15	0.69		0.05	0.83	0.75		0.05	336	200		14
S114	0.70	0.62		0.04	0.50	0.53		0.01				
H001	1.26	0.76		0.27	4.79	0.48		2.69	602	365		131
H006	2.76	1.37		0.22	3.18	1.36		0.32	410	204		33
H012	2.69	2.23		0.14	5.14	3.09		0.45	438	364		23
H032	3.27	1.84		0.28	3.95	2.38		0.32	457	257		39
H037	1.34	1.63		0.05	2.00	2.80		0.02				
H038	2.13	1.88		0.11	3.02	4.65		0.04	208	184		11
H048	1.32	0.90		0.11	1.23	1.02		0.08	137	93		12
H061	2.67	1.63		0.08	1.37	1.02		0.03	281	171		9
H095	3.28	2.80		0.21	4.79	6.06		0.12	403	344		26

[a] dw = dry weight

Table S5. Concentrations of atrazine and related compounds in natural sediments

Location	Waterbody	Sampling Year	Concentration Range	Reference
		Atrazine		
United States	Lake Michigan	2010-2011	N.D. to 6.18 ng/g	This study [a]
United States	Lake Superior	2011	N.D. to 1.85 ng/g	This study [a]
United States	Lake Huron	2012	N.D. to 3.28 ng/g	This study [a]
northeast China	Songhua River Basin	2010	N.D. to 40 ng/g	[6]
Beasley Lake Watershed, Sunflower County, Mississippi	agricultural drainage ditch	Before 2000	0.23 µg/g to 11 µg/g	[7]
Tarragona, Spain	Ebre Delta estuarine, top 10 cm	1990-1991	19.2 to 39.2 ng/g	[8]
Texas, New Mexico, and Oklahoma in U.S.	wetlands	2008-2009	< 2 ng/g to 37 ng/g	[9]
Northern Adriatic, Italy	Coastal lagoon	2004-2005	0.03-0.98 ng/g	[10]
German Bight	North Sea	1993	N.D.-0.50 ng/g [b]	[11]
Shelton, Nebraska	unknown	Before 1994	0.14 to 30.9 ng/g	[12]
		DEA		
United States	Lake Michigan	2010-2011	N.D. to 2.77 ng/g	This study [a]
United States	Lake Superior	2011	N.D. to 1.51 ng/g	This study [a]
United States	Lake Huron	2012	N.D. to 2.80 ng/g	This study [a]
Tarragona, Spain	Ebre Delta estuarine, top 10 cm	1990-1991	6.5 to 19.5 ng/g	[8]
German Bight	North Sea	1993	N.D. - 16 ng/g [b]	[11]
		Simazine		
United States	Lake Michigan	2010-2011	N.D. to 2.04 ng/g	This study [a]
Northern Adriatic, Italy	Coastal lagoon	2004-2005	N.D.-1.31 ng/g	[10]
German Bight	North Sea	1993	0.11 - 4 ng/g [b]	[11]
		Alachlor		
United States	Lake Michigan	2010-2011	N.D. to 0.61 ng/g	This study [a]
United States	Lake Superior	2011	N.D. to 0.13 ng/g	This study [a]
United States	Lake Huron	2012	N.D. to 0.77 ng/g	This study [a]
Northern Adriatic, Italy	Coastal lagoon	2004-2005	N.D.-1.75 ng/g	[10]

[a] Both Ponar and core surface (0-1 cm) segments are included.
[b] The wet weight based concentration is transformed to dry weight based concentration by assuming 90% water content.

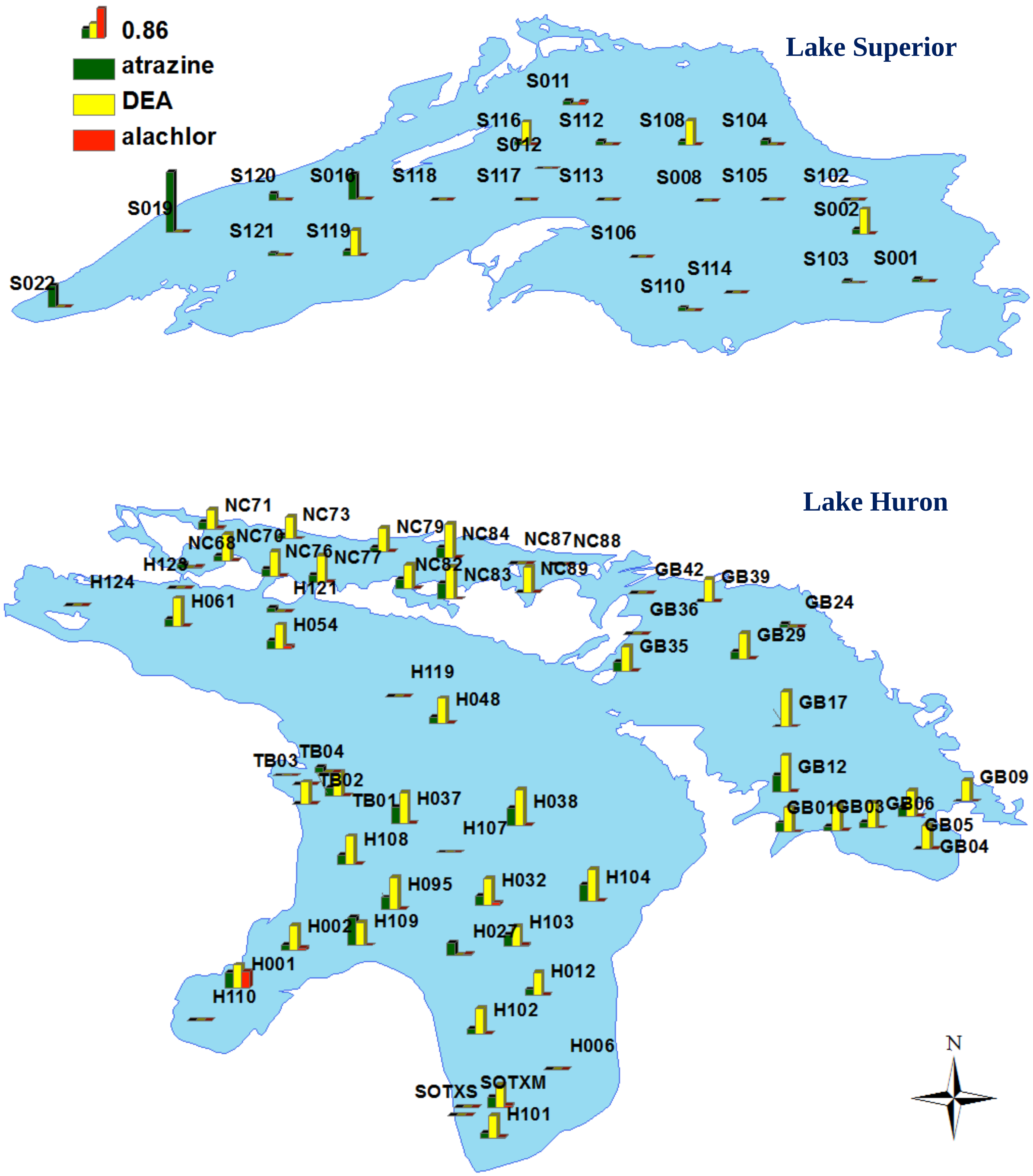


Figure S3. Spatial distribution of atrazine, DEA and alachlor concentrations (ng/g dw) in Ponar grab samples from Lake Superior and Lake Huron

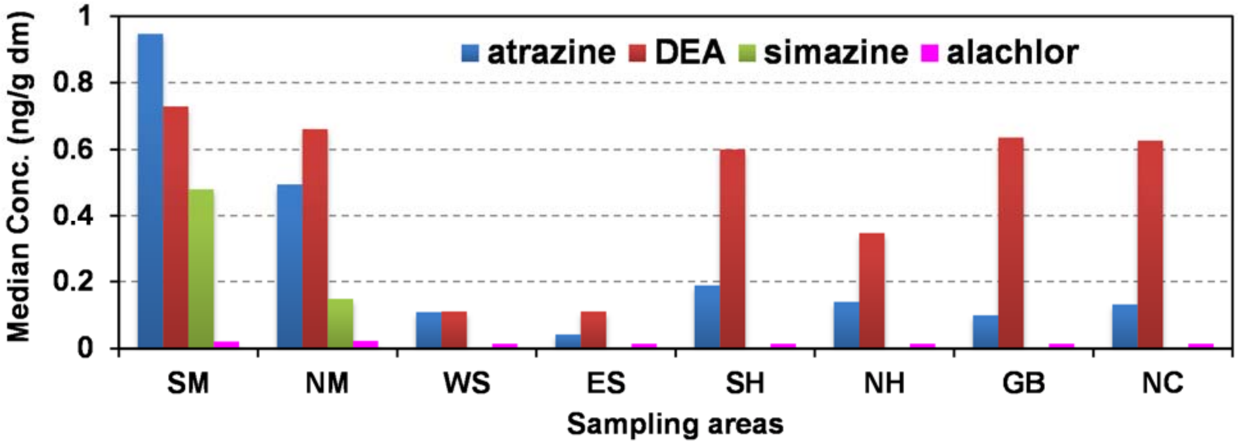


Figure S4. Comparison of median concentrations in Ponar grab samples among eight arbitrarily divided areas. See the Table below for abbreviations of the areas.

Table S6. Fisher's exact test for area comparison of chemical concentrations in Ponar grab samples. For each chemical, areas that do not share a letter are significantly different at 95% confidence level.

Area	Abbr.	N	atrazine	DEA	simazine	alachlor
southern Lake Michigan (<44°N)	SM	14	A	A	A	AB
northern Lake Michigan (>44°N)	NM	15	B	AB	B	AB
western Lake Superior (<87.573°W)	WS	12	C	C	BC	B
eastern Lake Superior (>87.573°W)	ES	12	D	C	B	B
southern Lake Huron (<44.4°N)	SH	16	CD	B	C	A
northern Lake Huron (>44.4°N)	NH	16	CD	B	C	B
Georgian Bay	GB	14	CD	B	C	B
The North Channel	NC	13	CD	B	C	B

Table S7. Pearson correlations among concentrations of target chemicals (natural log transformed) measured in PG sediments of Lakes Michigan, Superior and Huron for the concentrations above detection limits (N = 32)

		atrazine	**DEA**	**alachlor**	**simazine**
atrazine	r	1			
	p				
DEA	r	0.430	1		
	p	<.001			
alachlor	r	-0.045	0.197	1	
	p	0.805	0.296		
Simazine	r	0.760	0.631	0.181	1
	p	<.001	<.001	0.432	

Table S8. Averages (± S.D.) of net accumulation rate constant (k, y^{-1}), apparent doubling time (t_2, y), and the first order regression statistics (r and *p*) at coring sites of Lakes Michigan, Superior and Huron, obtained from fitting pseudo first order kinetics equation.

		atrazine	**DEA**	**simazine**
Lake Michigan	N	9	4	8
	k	0.027 ± 0.014	0.018 ± 0.008	0.027 ± 0.018
	t_2	33 ± 19	44 ± 20	42 ± 36
	r	0.979 ± 0.015	0.974 ± 0.015	0.953 ± 0.027
	p	<0.001	<0.001	0.001 ± 0.003
Lake Superior	N	8	5	
	k	0.016 ± 0.006	0.012 ± 0.006	
	t_2	48 ± 15	74 ± 44	
	r	0.943 ± 0.051	0.918 ± 0.057	
	p	0.026 ± 0.053	0.002 ± 0.002	
Lake Huron	N	7	6	
	k	0.018 ± 0.01	0.012 ± 0.007	
	t_2	62 ± 55	87 ± 78	
	r	0.954 ± 0.032	0.789 ± 0.112	
	p	<0.001	0.079 ± 0.153	

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