

Supporting Information

Comparison of GC-MS/MS and LC-MS/MS for the analysis of hormones and pesticides in surface waters: Advantages and pitfalls

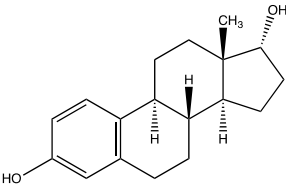
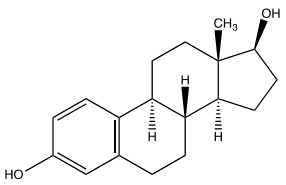
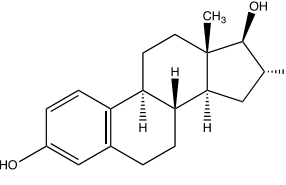
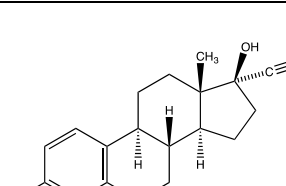
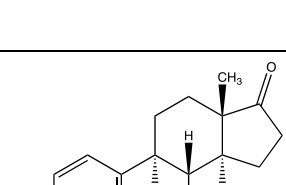
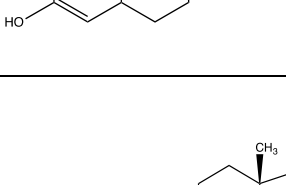
Ping He¹ and Diana S. Aga^{1*}

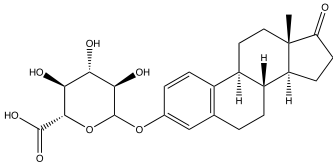
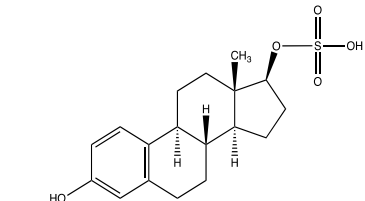
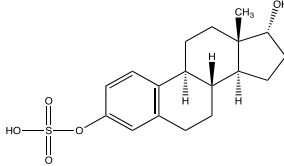
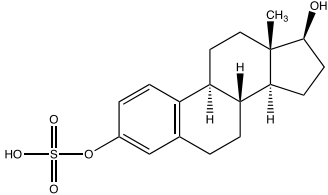
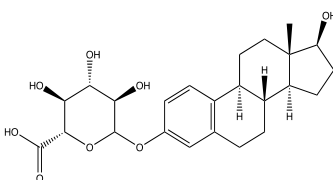
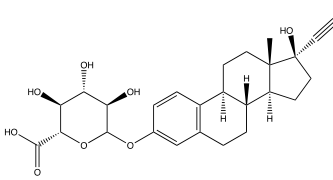
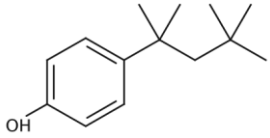
¹Department of Chemistry, University at Buffalo, The State University of New York, New York,
United States

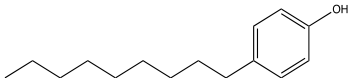
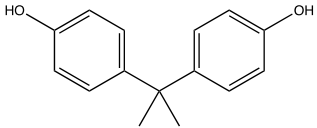
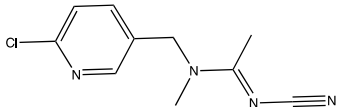
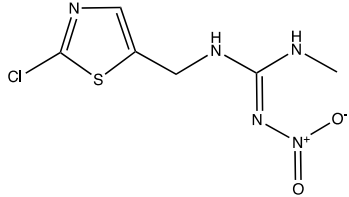
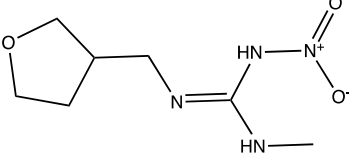
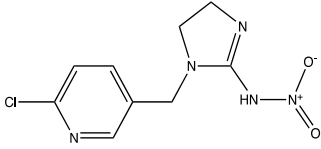
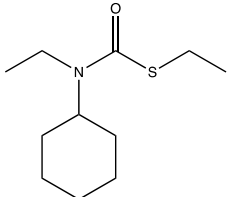
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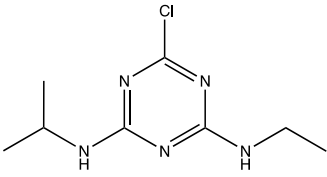
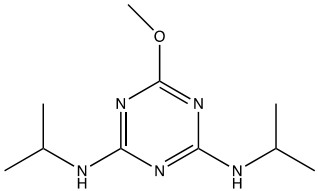
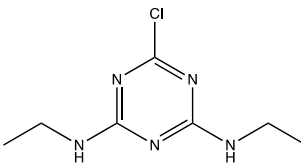
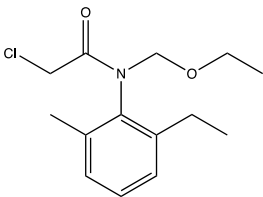
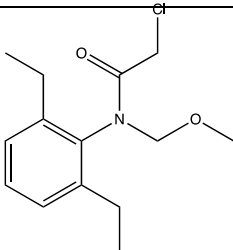
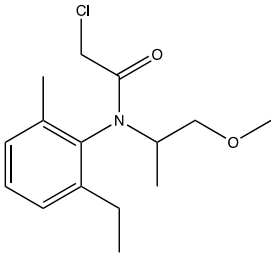
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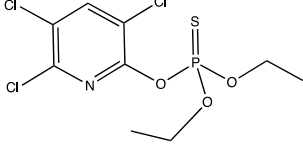
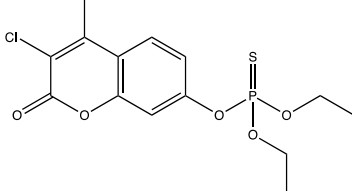
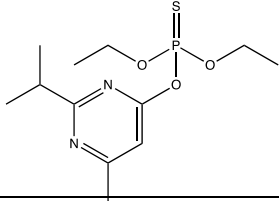
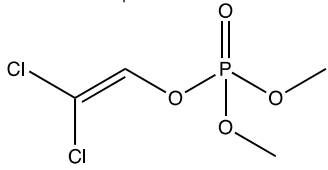
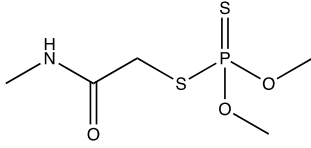
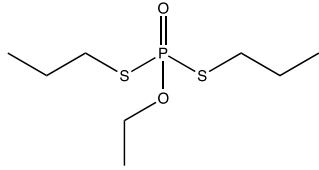
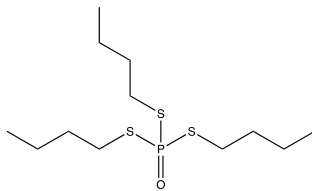
Table S1 Chemical structure and physico-chemical properties of the studied compounds.

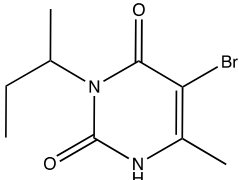
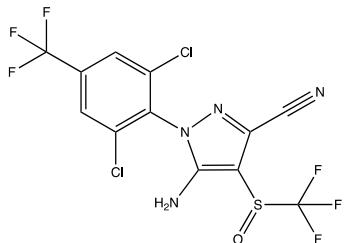
Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
17α-estradiol (E2α) 57-91-0 Free Estrogen		3.9 mg L ⁻¹ at 25 °C	4.01	10.33
17β-estradiol (E2β) 50-28-2 Free Estrogen		3.6 mg L ⁻¹ at 27 °C	4.01	10.33
17β-Estriol (E3) 50-27-1 Free Estrogen		27.34 mg L ⁻¹ at 25 °C	2.45	10.33
17α-Ethinylestradiol (EE2) 57-63-6 Free Estrogen		11.3 mg L ⁻¹ at 27 °C	3.67	10.33
Estrone (E1) 19973-76-3 Free Estrogen		30 mg L ⁻¹ at 25 °C	3.13	10.33
Estrone-3-sulfate (E1-3S) 481-97-0 Conjugated Estrogen		959.8 mg L ⁻¹ at 25 °C	2.5	-1.75

Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
Estrone-3-glucuronide (E1-3G) 2479-90-5 Conjugated Estrogen		172.5 mg L ⁻¹ at 25 °C	1.6	3.3
17β-estradiol-17-sulfate (β-E2-17S) 3233-69-0 Conjugated Estrogen		989.1mg L ⁻¹ at 25 °C	3.6	-1.36, 10.33
17α-estradiol-3-sulfate (α-E2-3S) 22139-70-4 Conjugated Estrogen		341.4 mg L ⁻¹ at 25 °C	2.1	-1.8
17β-estradiol-3-sulfate (β-E2-3S) 481-96-9 Conjugated Estrogen		341.4 mg L ⁻¹ at 25 °C	2.1	-1.8
17β-estradiol-3-glucuronide(β-E2-3G) 15270-30-1 Conjugated Estrogen		61.29 mg L ⁻¹ at 25 °C	1.1	3.3
17α-ethinylestradiol-3-glucuronide (EE2-3G) 60134-76-1 Conjugated Estrogen		30.72 mg L ⁻¹ at 25 °C	2.27	3.3
4-tert-octylphenol 140-66-9 Industrial compound		4.82 mg L ⁻¹ at 25 °C	5	10.23

Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
4-n-nonylphenol 104-40-5 Industrial compound		7 mg L ⁻¹ at 25 °C	5.76	10.31
Bisphenol A (BPA) 80-05-7 Industrial compound		300 mg L ⁻¹ at 25 °C	3.32	9.78
Acetamiprid 135410-20-7 neonicotinoid		4.25 × 10 ³ mg L ⁻¹ at 25 °C	0.8	-0.27, 4.16 (basic pKa)
Clothianidin 210880-92-5 neonicotinoid		327 mg L ⁻¹ at 20 °C	0.7	10.8 (acidic pKa) 7.09 (basic pKa)
Dinotefuran 165252-70-0 neonicotinoid		5.43 × 10 ⁴ mg L ⁻¹ at 20 °C	-0.644	10.85 (acidic pKa) 7.99 (basic pKa)
Imidacloprid 138261-41-3 neonicotinoid		6.1 × 10 ² mg L ⁻¹ at 20 °C	0.57	10.6 (acidic pKa) 6.75 (basic pKa)
Cycloate 1134-23-2 thiocarbamate		85 mg L ⁻¹ at 22 °C	3.88	NA ⁴

Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
Atrazine 1912-24-9 triazine		34.7 mg L ⁻¹ at 26 °C	2.61	14.48 (acidic pKa) 4.2 (basic pKa)
Prometon 1610-18-0 triazine		750 mg L ⁻¹ at 20 °C	2.99	14.27 (acidic pKa) 5.97 (basic pKa)
Simazine 122-34-9 triazine		6.2 mg L ⁻¹ at 20 °C	2.18	14.75 (acidic pKa) 4.23 (basic pKa)
Acetochlor 34256-82-1 chloroacetamide		233 mg L ⁻¹ at 25 °C	4.14	NA
Alachlor 15972-60-8 chloroacetamide		240 mg L ⁻¹ at 25 °C	3.52	NA
Metolachlor 51218-45-2 chloroacetamide		488 mg L ⁻¹ at 25 °C	3.13	NA

Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
Chlorpyrifos 2921-88-2 organophosphorus		1.4 mg L ⁻¹ at 25 °C	4.96	NA
Coumaphos 56-72-4 organophosphorus		1.5 mg L ⁻¹ at 20 °C	4.13	NA
Diazinon 333-41-5 organophosphorus		40 mg L ⁻¹ at 25 °C	3.81	NA
Dichlorvos 62-73-7 organophosphorus		8000 mg L ⁻¹ at 25 °C	1.43	NA
Dimethoate 60-51-5 organophosphorus		2.5 × 10 ⁴ mg L ⁻¹ at 25 °C	0.78	NA
Ethoprop 13194-48-4 organophosphorus		22.41 mg L ⁻¹ at 25 °C	3.6	NA
Tribufos 78-48-8 organophosphorus		2.3 mg L ⁻¹ at 20 °C	5.7	NA

Analyte CAS number Class	Structure	Water Solubility ¹	LogP (at 25 °C) ²	pKa ³
Bromacil 314-40-9 substituted uracils		815 mg L ⁻¹ at 25 °C	2.11	9.95
Fipronil 120068-37-3 phenylpyrazole		1.9 mg L ⁻¹ at 20 °C	4	NA

¹ Water solubility value from Pubchem database

² LogP value from Chemspider database using predicted data generated using the US Environmental Protection Agency's EPISuite™

³ pKa value are structure-based predictions from Chemicalize database

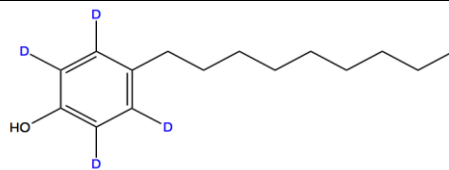
⁴ NA: value not available

Table S2 List of surrogate compounds in this study

Surrogate compound	Structure
Estrone-2,4,16,16-d ₄ (E1-d ₄)	
17β-Estradiol-16,16,17-d ₃ (E2-d ₃)	
Ethinylestradiol-2,4,16,16-d ₄ (EE2-d ₄)	
Estrone-3-sulfate-2,4,16,16-d ₄ (E1-3S-d ₄)	
17β-Estradiol-3-sulfate-2,4,16,16-d ₄ (E2-3S-d ₄)	
17β-Estradiol-3-glucuronide-16,16,17-d ₃ (E2-3G-d ₃)	

Dinotefuran-d3	
Atrazine-d5	
Prometon-d14	
Metolachlor-d6	
Acetochlor-d11	
Chlorpyrifos-d10	
Diazine-d10	

4-NP-d4



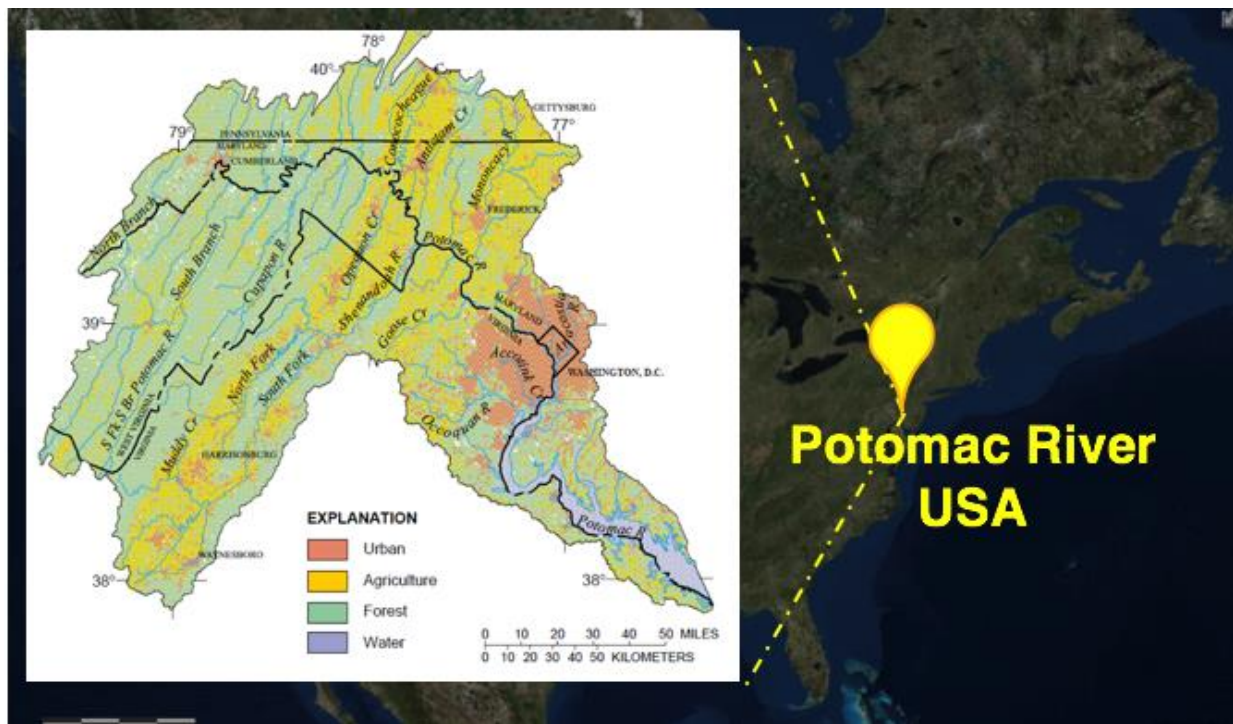


Figure S1. Map of the Potomac River watershed. (The authors would like to thank Erik Rosenfeldt for drawing the map in this Figure)

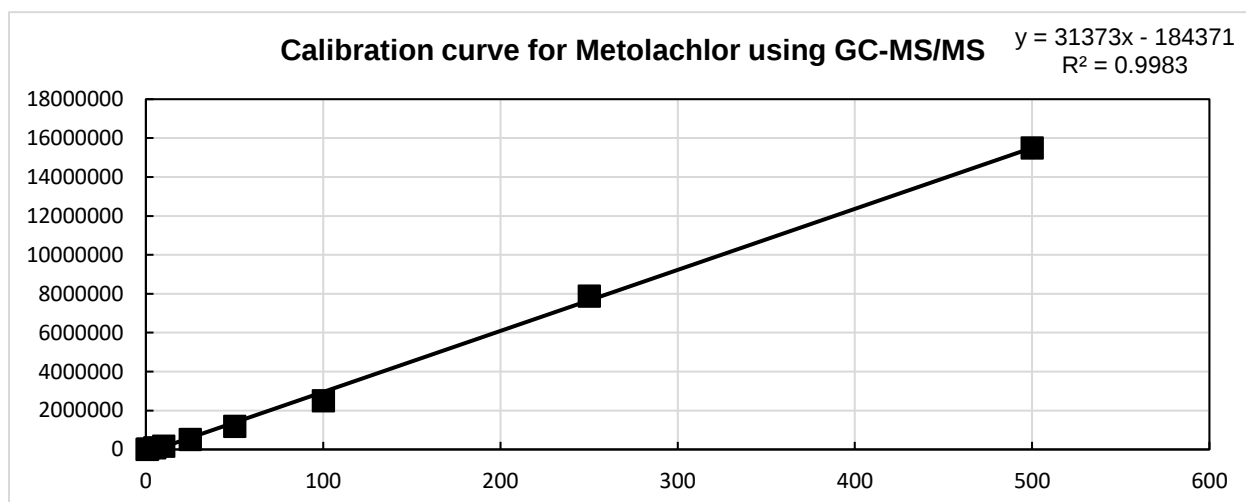
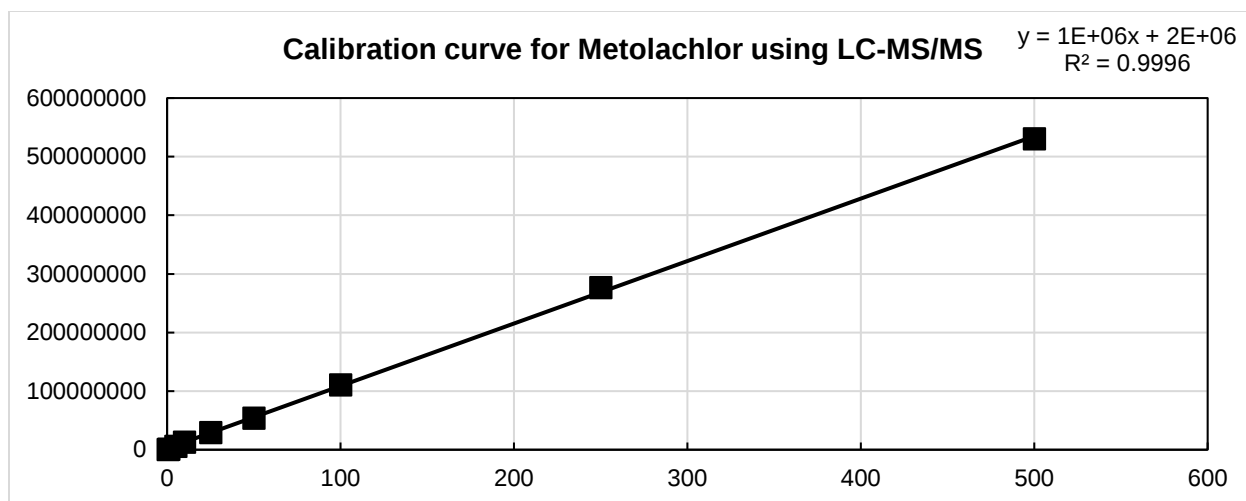


Figure S2. Example of calibration curves for metolachlor using LC-MS/MS and GC-MS/MS

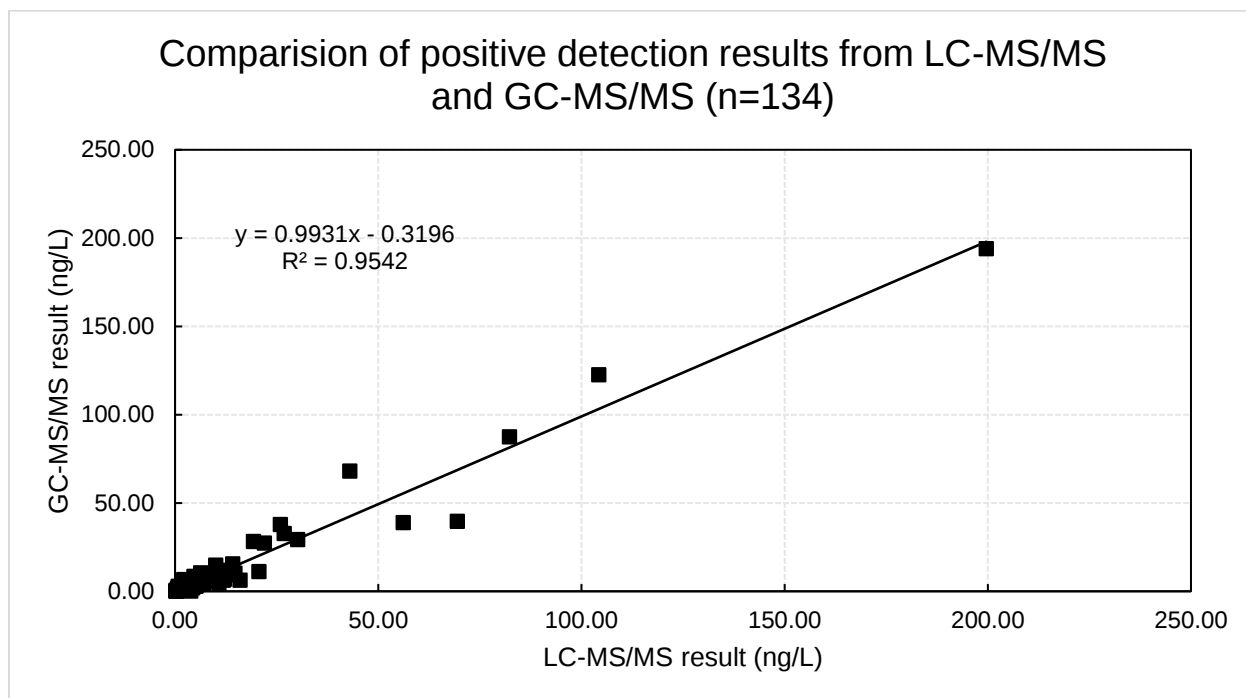


Figure S3. Comparison of positive detection results determined by GC-MS/MS and LC-MS/MS from 35 water samples.

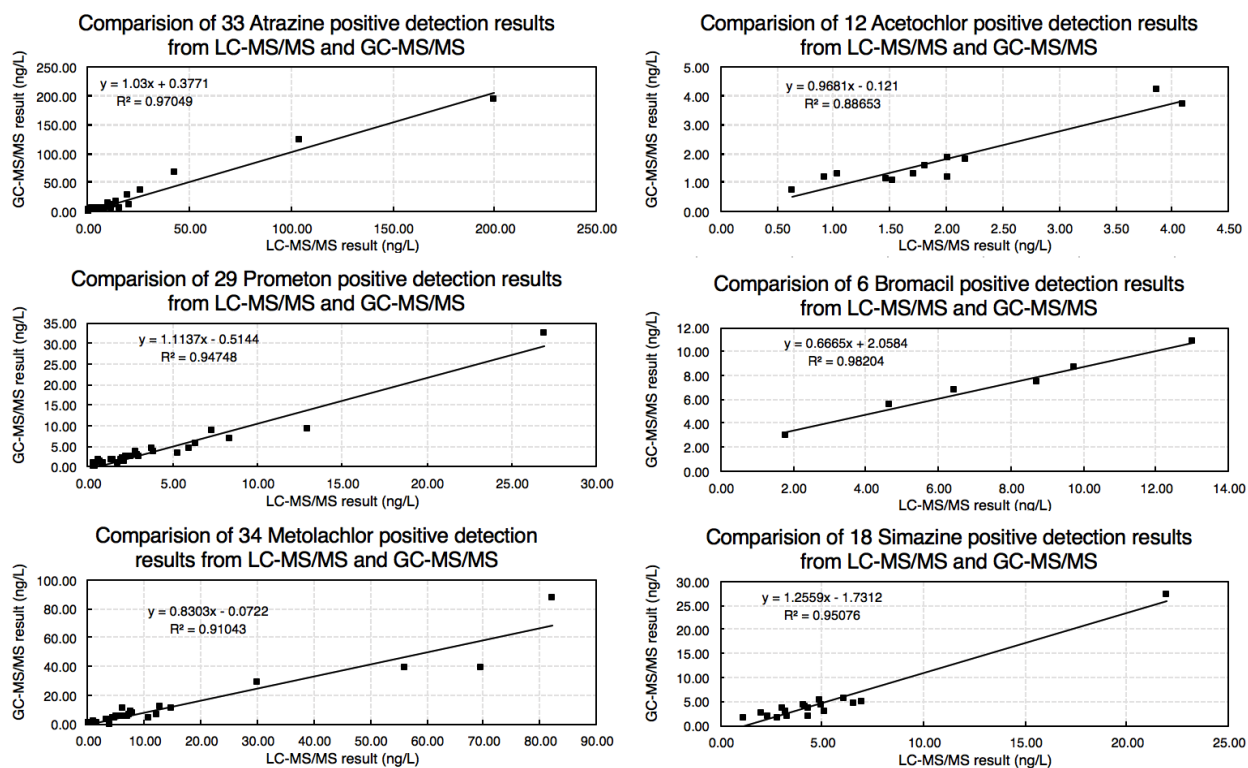


Figure S4. Individual comparison of positive detection results determined by GC-MS/MS and LC-MS/MS from 35 water samples. Note only two samples have Alachlor detected therefore not presented in individual comparison.

