

Pharmaceuticals and Personal Care Products in Minnesota's Rivers and Streams: 2010



Minnesota Pollution Control Agency

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Executive Summary

In 2010, the Minnesota Pollution Control Agency (MPCA), with guidance from the U.S. Environmental Protection Agency (EPA), conducted a probabilistic survey of Minnesota's flowing waters. Probabilistic surveys, which are based on randomly selected sampling locations to give statistically valid water quality information, are an important part of Minnesota's surface water monitoring system in conjunction with its Intensive Watershed Monitoring program. Analysis of eighteen pharmaceuticals and personal care products (PPCPs) was done on water samples collected at 150 locations included in this study. These chemicals, some of which possess endocrine active properties, are of increasing interest as unregulated contaminants in Minnesota's surface water.

The results of this study show that:

- Parabens, which are used as preservatives for food and cosmetics, are commonly present in the surface water of rivers and streams, with methyl paraben detected in over 30 percent of the samples.
- Benzotriazole, a corrosion inhibitor, was found in 6 percent of the samples, while methylbenzotriazole, a degradation product of benzotriazole, was detected in 12 percent of the samples.
- The anticonvulsant medication carbamazepine was detected in 6 percent of the samples.
- Antidepressant pharmaceuticals were commonly present, with venlafaxine found in 9 percent of the water samples.

Background

Improvements in analytical methods have allowed us to detect the presence of contaminants in surface water at ever lower concentrations. Whereas the limits of detection for most contaminants were in the parts per million 35 years ago, it is typical now for contaminants to be reported at the part per trillion concentrations.

The ability to detect contaminants at these very low concentrations has paralleled the growing understanding that particular chemicals pose dangers to organisms not because they are necessarily toxic at high concentration, but because they have adverse, hormone-like effects at exceedingly low concentration (Streets et al. 2008). Several studies have now shown that these *endocrine active chemicals* (EACs) and other bioactive chemicals can alter fish behavior (Painter et al. 2009), reproductive biology, and populations (Kidd et al. 2007) at part per trillion concentrations. The presence of these chemicals in water at low levels is not, therefore, simply a matter of low-level detection, but constitutes a real concern for ecosystems and possibly for human health.

Previous field studies have demonstrated that PPCPs and other unregulated commercial or industrial chemicals are surprisingly widespread in our aquatic environment. The USGS monitoring of pharmaceuticals, hormones, and other chemicals in United States waters in 2002 (Kolpin et al. 2002) and in Minnesota (Lee et al. 2004) revealed that alkylphenols, hormones, plasticizers, and other chemicals were often present in rivers. Subsequent monitoring studies in the Mississippi River and its tributaries (Lee et al. 2008a; Lee et al. 2008b) yielded similar results, along with evidence of endocrine disrupting effects in fish collected at those water sampling locations.

Most of these studies focused on the impact of wastewater treatment plant (WWTP) effluent, being a predominant source of unregulated contaminants to aquatic ecosystems. Considerably less work has been done on a random sampling of lakes and rivers on a large scale to ascertain the presence of PPCPs in water not directly affected by WWTP effluent. The National Flowing Waters Survey presented an opportunity to collect water from 150 river locations selected at random from across Minnesota. The results of that analysis are reported here. The data reveal that several PPCPs and other chemicals are routinely detected in Minnesota's waterways at low concentration.

Sampling and analysis methods/approach

Surface water samples were collected at 150 randomly selected sites from all three of Minnesota's ecological regions (Figure 1). Using a GIS map that contains river lines called NHD-Plus, sites were randomly selected using a statistical program that selects points based on the location of those river lines and stream size. After site points were generated along with latitude and longitudinal coordinates, site locations were verified in the field as acceptable sampling locations. Figure 1 illustrates the general locations of where these sites were sampled once they had been verified.

Water samples were analyzed for eighteen PPCPs by the Minnesota Department of Health Laboratory (Table 1). Some of these analytes, such as the anticonvulsive medicine carbamazepine and the antidepressant fluoxetine, have been monitored and detected previously in Minnesota's surface water (Lee et al. 2010). Parabens and artificial sweeteners (saccharine and acesulfame) have not been monitored in Minnesota's surface water previously.

Collecting data from randomly selected stream sites reduces bias and allows information gathered from a few sites to be extrapolated to the entire stream network. Site selection was stratified by level II ecoregion which roughly divides the state into three sectors: a northern region known as the Mixed Wood Shield (MWS), the Mixed Wood Plains (MWP) in the center, and the Temperate Prairies (TP) in the south and up the western border of the state. Each region encompasses different land uses, ecological structures, and geological composition. Approximately 50 sites were sampled in each of these three ecoregions totaling 150 throughout the state.

Once PPCP samples had been analyzed, samples were categorized as either detected or non-detected for each chemical. Condition estimates of stream miles were calculated for each PPCP utilizing the categorical analysis function with a statistical program (Kincaid 2013). The categorical analysis function calculates the proportion and size of each chemical within each ecological region.

Results

Methyl and propyl parabens were the most frequently detected chemicals in this study, found in 32 percent and 21 percent of the samples, respectively. Methyl paraben was found at a maximum concentration of 1000 ng/L, while propyl paraben was found up to 600 ng/L.

Methylbenzotriazole, a degradation product of the anticorrosive chemical benzotriazole, was found in 12 percent of the samples up to 1,080 ng/L, while benzotriazole was detected at 6 percent of the locations at a maximum of 1,240 ng/L (Figures 2, 3).

Carbamazepine, a commonly prescribed medication in the treatment of attention deficit hyperactivity disorder (ADHD), was found in 6 percent of the samples at concentrations up to 34 ng/L.

Five antidepressant medications (SSRIs, or selective serotonin re-uptake inhibitors) were analyzed. Venlafaxine was the most commonly detected SSRI, found in 9.4 percent of the water samples. This was followed by citalopram, sertraline, and bupropion, found in 4, 2.7, and 2 percent of the samples, respectively. Fluoxetine was detected in one sample. Of the SSRIs, venlafaxine was detected at the highest concentration, at 34 ng/L. Norsesertraline, a degradation product of sertraline, was found in 2.6 percent of the samples at a maximum concentration of 43.1 ng/L.

Gemfibrozil, a cholesterol-lowering medication, was found at 12 locations, representing 8 percent of the samples, at a maximum concentration of 131 ng/L. The artificial sweeteners saccharine and acesulfame were each detected at one sampling location.

Figures 4 – 21 show the calculated estimated stream mile percentage for each PPCP within each ecoregion as well as the statewide calculation of stream miles with detectable levels of PPCPs.

Discussion

In a broad sense, the results of this study confirm those of other investigations over the past decade that revealed that pharmaceuticals, personal care products, and other unregulated chemicals are commonly present in surface water across Minnesota. However, while prior studies have tended to focus on particular sources of these contaminants to the aquatic environment, such as WWTPs, this large-scale investigation shows that several pharmaceuticals and other chemicals are present in rivers or streams lacking obvious, proximate sources of contamination.

Although parabens, which are widely used as preservatives in cosmetics, pharmaceuticals, and foods, are not considered toxic, they are reportedly weakly estrogenic (Routledge et al. 1998). Based on the results of this study, parabens are apparently quite widespread in Minnesota's surface water: methyl paraben and propyl paraben were detected at over 30 percent and 20 percent of the sampling locations, respectively, (Figure 3), both at concentrations that approached 1000 ng/L (1 ppb) (Figure 2).

Carbamazepine, a medication used in the treatment of ADHD, has been detected frequently in surface waters at low concentrations. In an earlier Minnesota study of WWTPs, carbamazepine was found in 5 percent of the water samples collected *upstream* of the outfall locations of treatment plants. In this study, carbamazepine was detected at a similar frequency of 6 percent. Currently, there are no reported adverse effects of carbamazepine at part per trillion concentrations on fish or wildlife. However, because it is a very biologically active chemical there is concern that it may have some unknown adverse environmental effect.

Similarly, SSRI antidepressant medications are commonly found in surface waters (Schultz and Furlong 2008). In this study, the SSRIs venlafaxine, fluoxetine, sertraline, citalopram, and bupropion were all detected in surface water. The most frequently detected antidepressant was venlafaxine, found in over 9 percent of the samples. This frequency of detection is consistent with previous investigations, when it was detected in 6 percent of water collected upstream of WWTP outfalls. Research has shown that fish behavior (Painter et al. 2009) and freshwater mussel reproduction (Fong 1998) is altered by antidepressants at low part per trillion concentrations.

Benzotriazole is a widely used corrosion inhibitor in aircraft de-icers and anti-ice fluids, antifreeze, hydraulic fluids, and for silver protection in dishwasher detergents. Approximately 9,000 tons of benzotriazole are produced in the United States annually. Aircraft de-icers and anti-ice fluids contains up to 1.7 percent benzotriazole, while dishwasher detergent contains up to 27 milligrams per wash load (Janna et al. 2011; Wolschke et al. 2011). It is only partially removed in WWTPs, is very resistant to

degradation, and highly persistent in the aquatic environment (Breedveld et al. 2003; Harris et al. 2007). It was found in 6 percent of the samples collected for this study, and together with methyl benzotriazole - a degradation product of benzotriazole - is one of the more commonly detected unregulated contaminants in Minnesota's surface water. The widespread occurrence of this chemical in Minnesota's surface water is consistent with what is reported in other studies (Giger et al. 2006; Voutsas et al. 2006).

While little chronic toxicity data is available on which to base a sound ecological risk assessment of benzotriazole, it is highly toxic to plants at 100 parts per billion and is acutely toxic to fish in the low part per million range (Wu et al. 1998). *In vitro* assays conducted using a recombinant yeast (anti-)estrogen assay indicated that benzotriazole possessed anti-estrogenic properties (Harris et al. 2007).

Benzotriazole and methylbenzotriazole, were detected at a concentration of over 1 part per billion in this study. Benzotriazole concentrations in primary and secondary effluents of municipal wastewater treatment plants has been reported up to 100 g/L (Voutsas et al. 2006). In winter, with higher usage of de-icing solutions, concentrations of benzotriazole may well exceed concentrations considered safe for aquatic organisms (Seeland et al. 2012).

Artificial sweeteners and caffeine are often detected in surface and groundwater. These are obviously not toxic to humans, but are ideal chemical tracers for wastewater due to their mobility and persistence in the environment (Van Stempvoort et al. 2011). In this study, saccharine and acesulfame were reported in less than 1 percent of the samples.

Condition estimate evaluations

A study of this magnitude focusing on pharmaceuticals and other unregulated contaminants in surface water is unusual. The size of the study, coupled with the randomized approach to selecting sample locations, makes it possible to statistically evaluate the extent that rivers in Minnesota are affected by the chemicals that were detected in the investigation. "Condition estimates" that are based on statistical evaluations of the data collected in this randomized study are useful in understanding the degree to which individual chemicals may be found in rivers and streams across the state.

Figures 4 through 21 show the estimated percentages of stream miles in Minnesota with detectable concentrations of the chemicals analyzed in this study, separated into the three major ecological regions of the state (Figure 1). The MWS, typified with abundant wetlands, lakes, and forests, has relatively little urban or agricultural development when compared to either the MWP or the TP regions. The TP region is influenced more than the MWP by agricultural activity and human disturbance, though the estimated urban influence is almost indistinguishable between these two regions.

The condition estimates shown in Figures 4 through 21 indicate that the TP and MWP ecological regions have the greatest number of stream miles with detectable concentrations of the chemicals analyzed in this study. Similar patterns of occurrence are observed with nitrogen and phosphorus (data not shown), and is likely correlated to the degree these regions are influenced by various forms of agriculture and urban development. For most of these chemicals, the MWS appears to have the lowest number of affected stream miles.

Potential impacts

Although the impacts that these chemicals have on fish and wildlife at the concentrations reported here are largely unknown, a growing body of evidence suggests that some unregulated contaminants may be exerting adverse effects on aquatic ecosystems in subtle but still undocumented ways. Studies involving mixtures of pharmaceuticals frequently found in surface water have been observed to alter genetic expression in embryonic cells (Pomati et al. 2006) and fish cells (Pomati et al. 2007) at the concentrations typically found in surface water investigations.

Several of the unregulated contaminants detected in surface water over several years of investigation are either known or suspected endocrine active chemicals. These include, but are not limited to, hormones, alkylphenols, bisphenol A, and particular pesticides or herbicides that are capable of eliciting hormone-like effects on organisms at part per trillion concentrations. The discovery that vitellogenin - the egg-related protein normally produced in female fish - is also produced in males suggests that fish are frequently exposed to endocrine active chemicals in lakes and streams (Writer et al. 2010). Other investigations examining the effect of endocrine active chemicals on fish show clear and sometimes dramatic effects on the behavior, population, and the genetic expression of aquatic organisms at concentrations that are similar to those reported here.

This survey of 150 flowing surface water locations in Minnesota is part of an ongoing effort to document the presence of unregulated contaminants in the state's lakes, rivers, and streams. Analysis of PPCPs and EACs is planned for future probabilistic surveys of Minnesota lakes and flowing waters on a five year rotating basis. Data collected over time from these studies will provide a clearer picture of the types and frequency of unregulated contaminants in the aquatic environment.

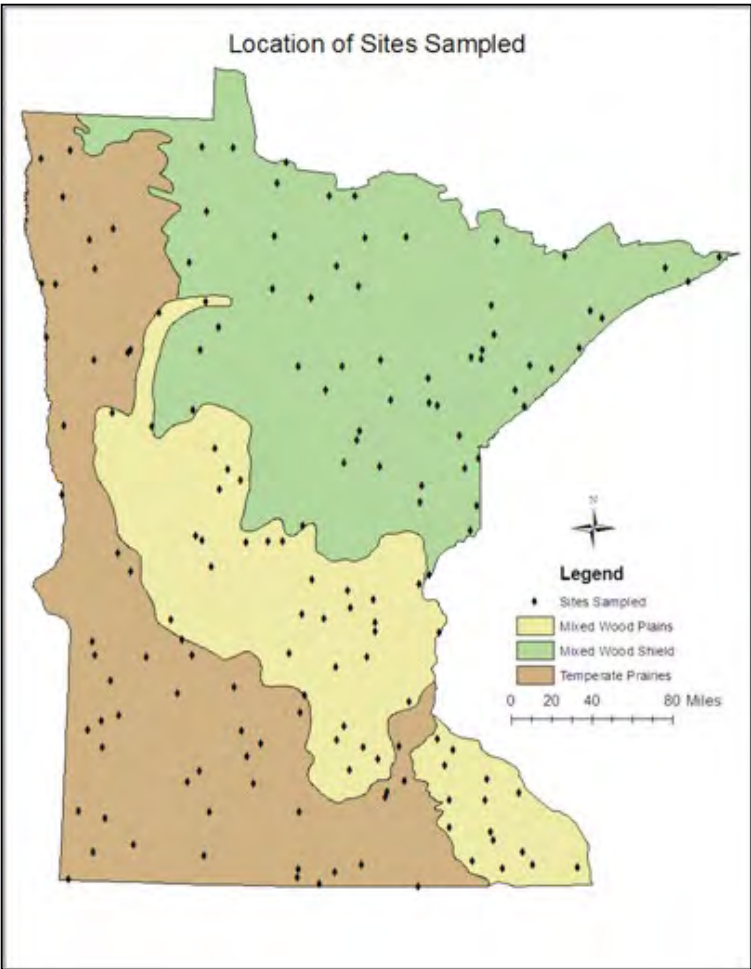


Figure 1. Surface water sampling locations within each of Minnesota’s three ecological regions.

Table 1. Name and descriptions of chemicals analyzed for the study.

Chemical	Description
Benzotriazole	Corrosion inhibitor
Methylbenzotriazole	Degradation product of benzotriazole
Ethyl paraben	Preservative for foods and pharmaceuticals
Propyl paraben	Preservative for foods and pharmaceuticals
Butyl paraben	Preservative for foods and pharmaceuticals
Benzyl paraben	Preservative for foods and pharmaceuticals
Acesulfame	Food additive; artificial sweetener
Saccharine	Food additive; artificial sweetener
Bupropion	Pharmaceutical; an antidepressant
Citalopram	Pharmaceutical; an antidepressant
Carbamazepine	Pharmaceutical; an anticonvulsant
Gemfibrozil	Pharmaceutical; a lipid regulator
Fluoxetine	Pharmaceutical; an antidepressant
Norfluoxetine	An active metabolite of fluoxetine
Sertraline	Pharmaceutical; an antidepressant
Norsertaline	An active metabolite of sertraline
Venlafaxine	Pharmaceutical; an antidepressant

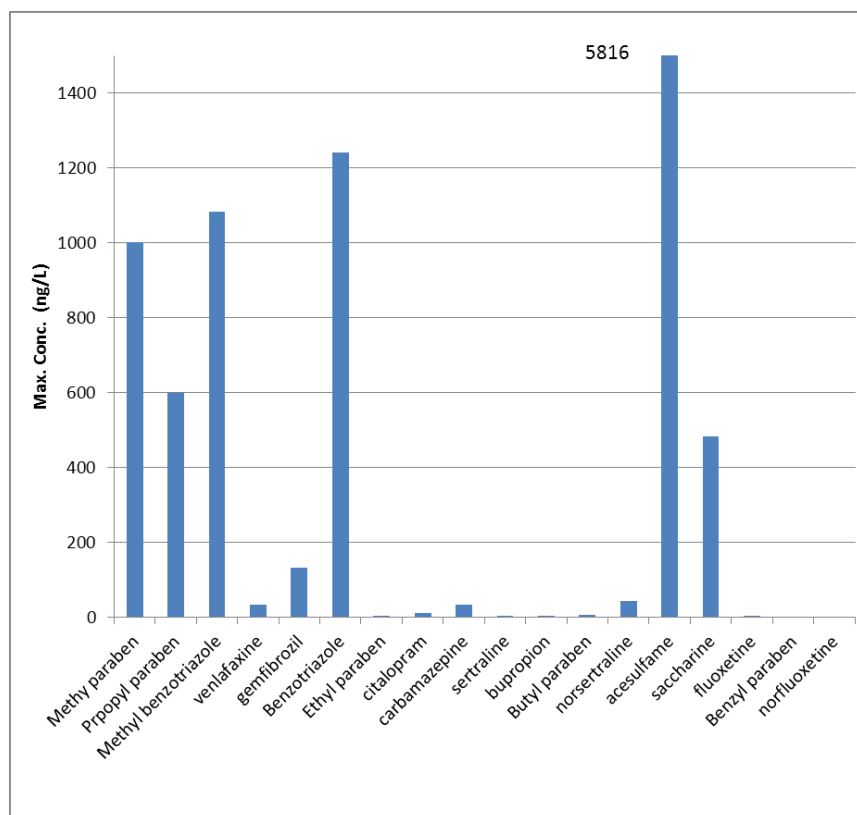


Figure 2. Maximum concentrations of chemicals detected in the samples collected from 150 randomly selected river locations in Minnesota.

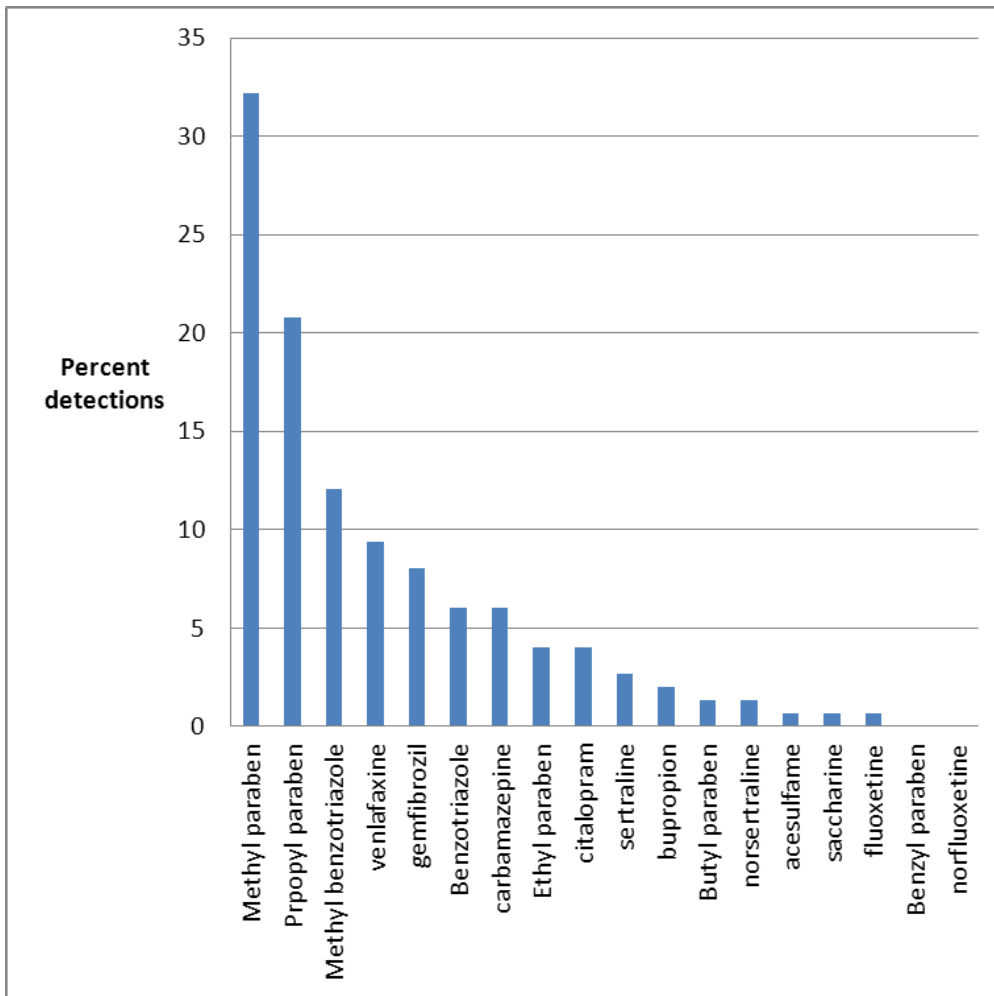


Figure 3. The percent of river surface water samples with detections of the chemicals analyzed in this study of 150 randomly selected locations in Minnesota.

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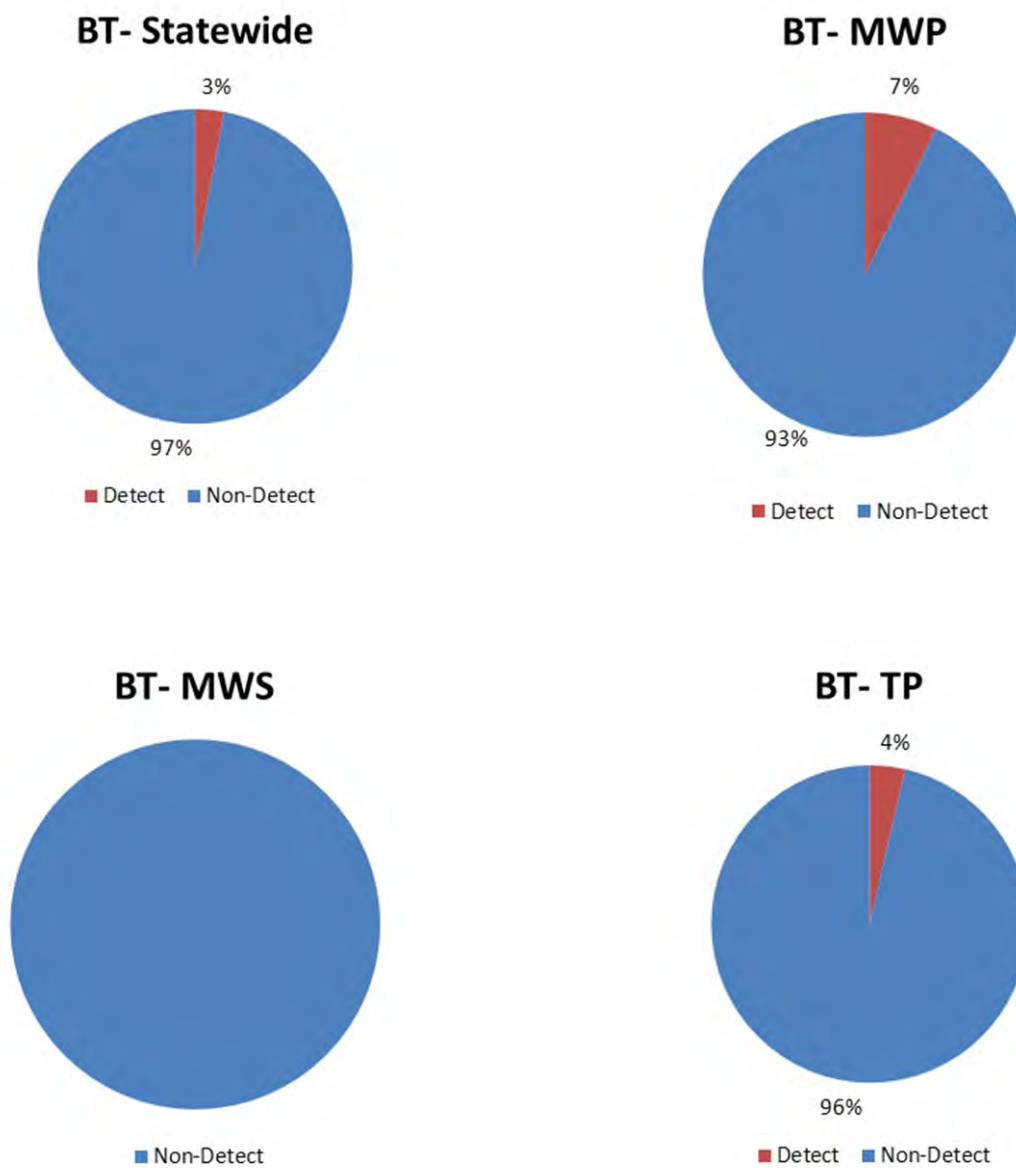


Figure 4. Estimated percentage of stream miles with detectable concentrations of benzotriazole across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

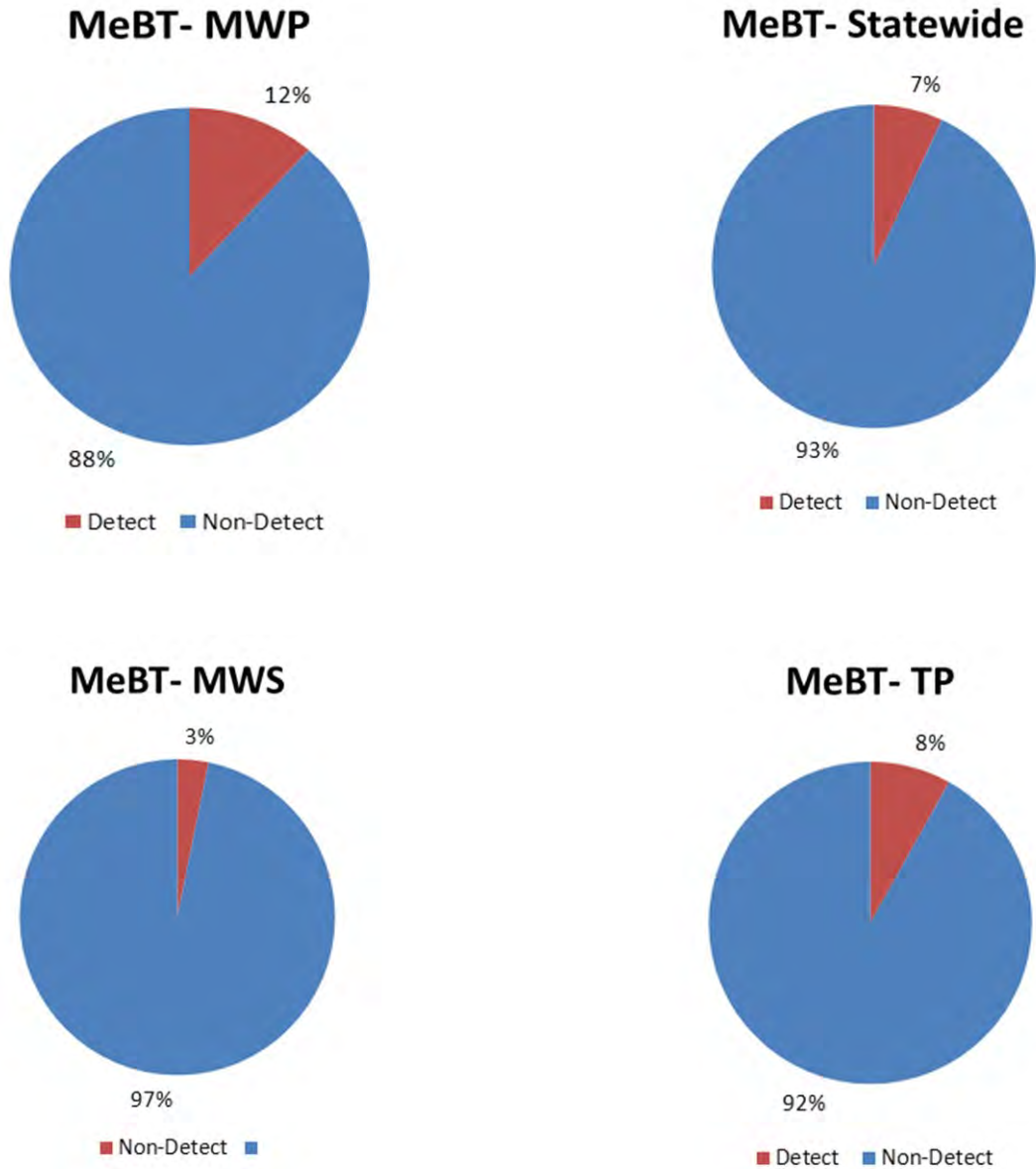


Figure 5. Estimated percentage of stream miles with detectable concentrations of methylbenzotriazole across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

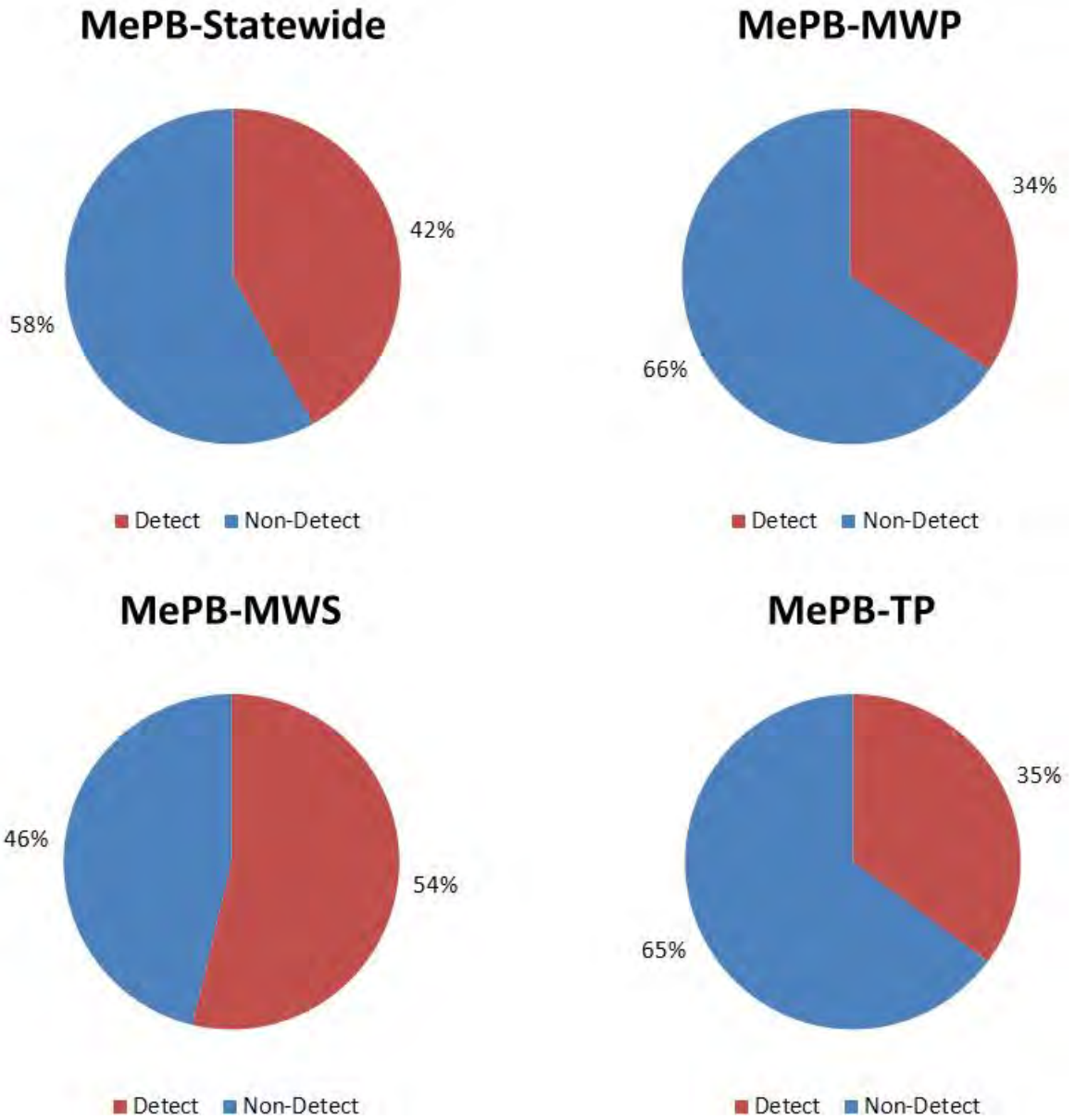


Figure 6. Estimated percentage of stream miles with detectable concentrations of methylparaben across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

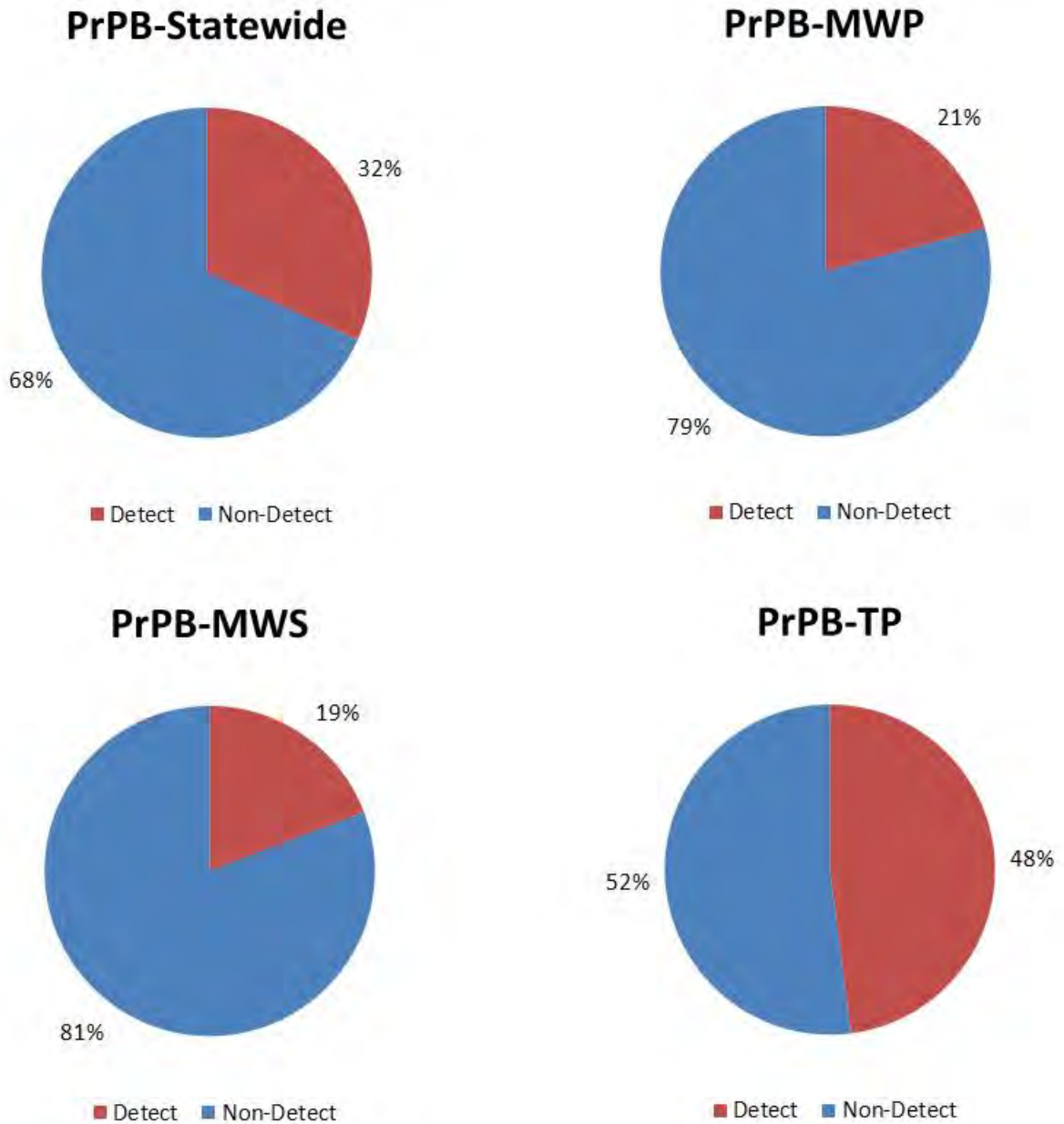
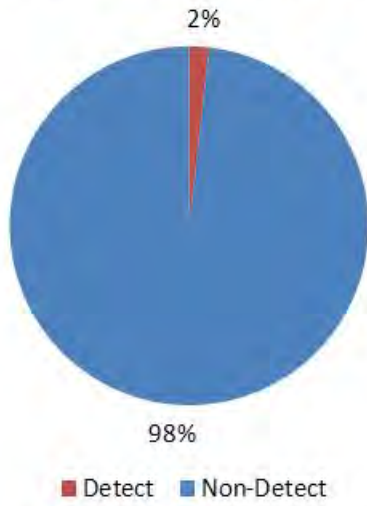


Figure 7. Estimated percentage of stream miles with detectable concentrations of propylparaben across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

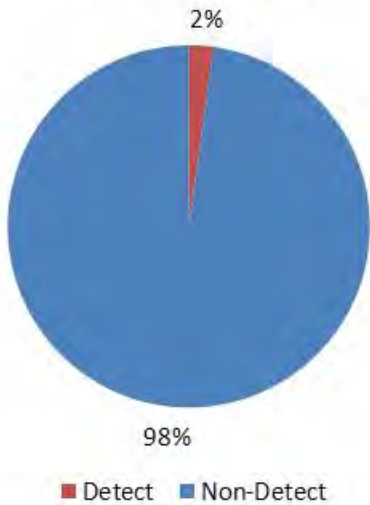
BuPB-Statewide



BuPB-MWP



BuPB-MWS



BuPB-TP

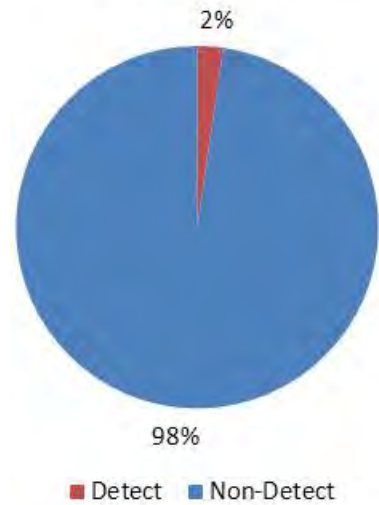


Figure 8. Estimated percentage of stream miles with detectable concentrations of butylparaben across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

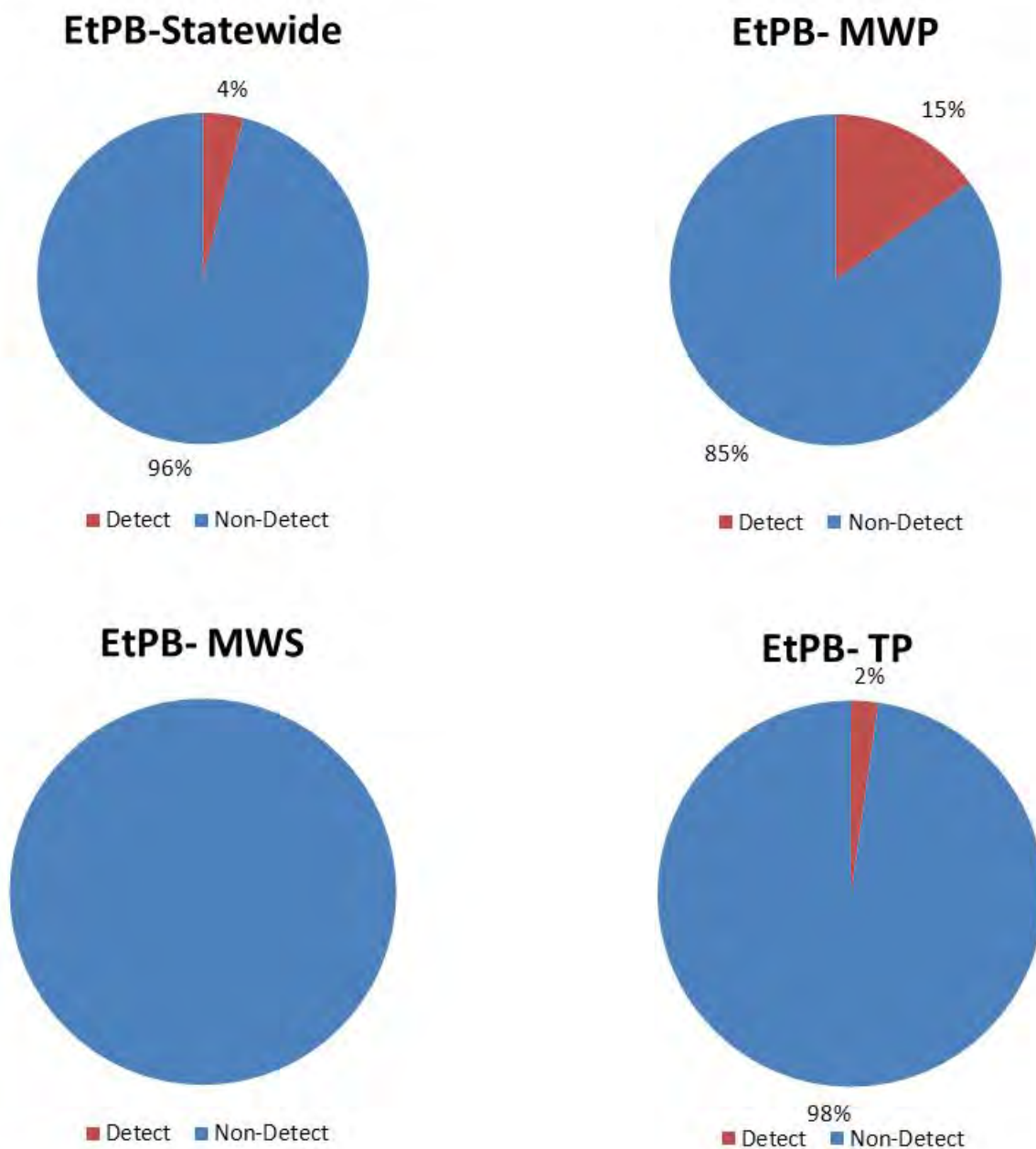


Figure 9. Estimated percentage of stream miles with detectable concentrations of ethylparaben across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

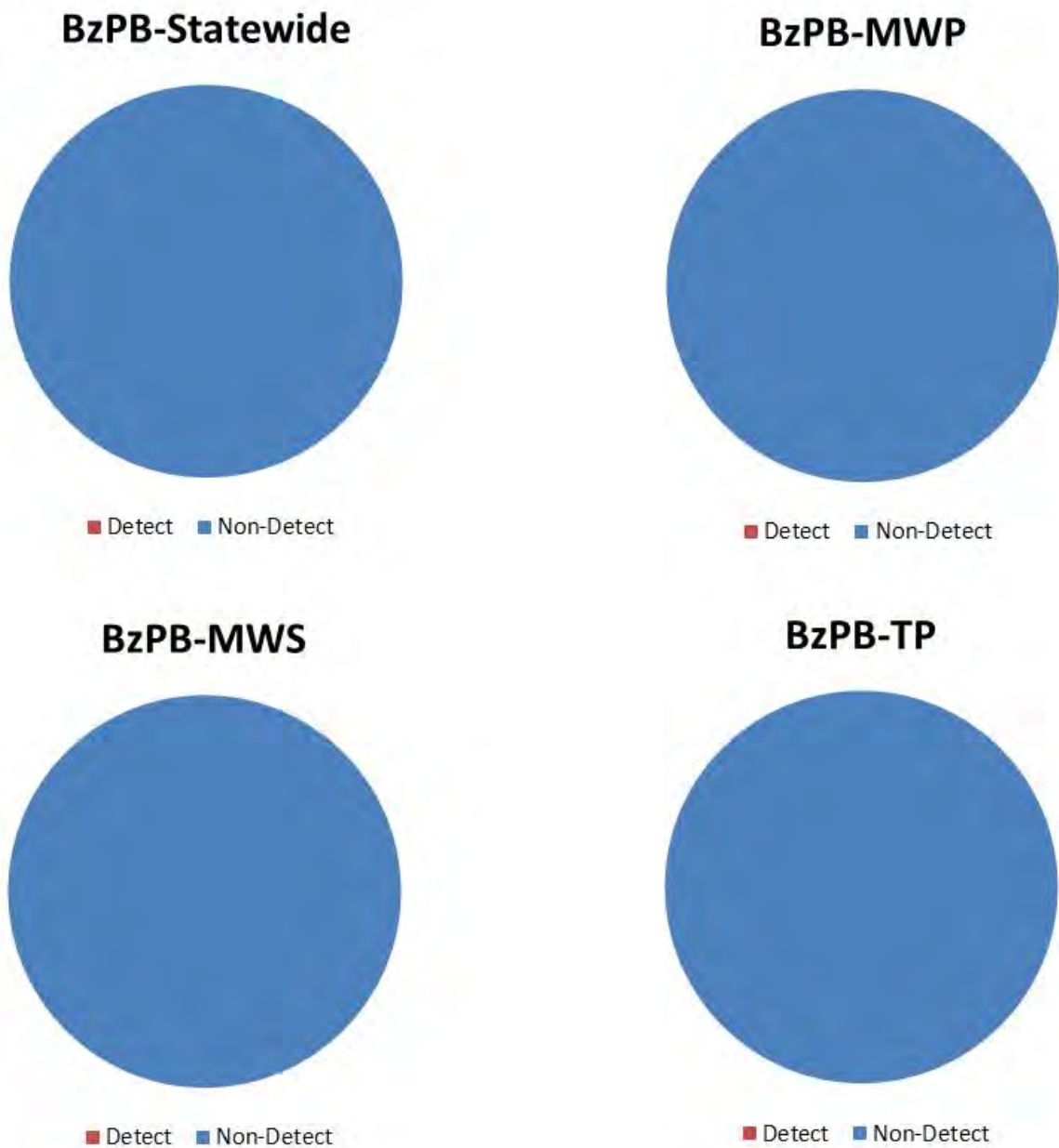


Figure 10. Estimated percentage of stream miles with detectable concentrations of benzylparaben across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

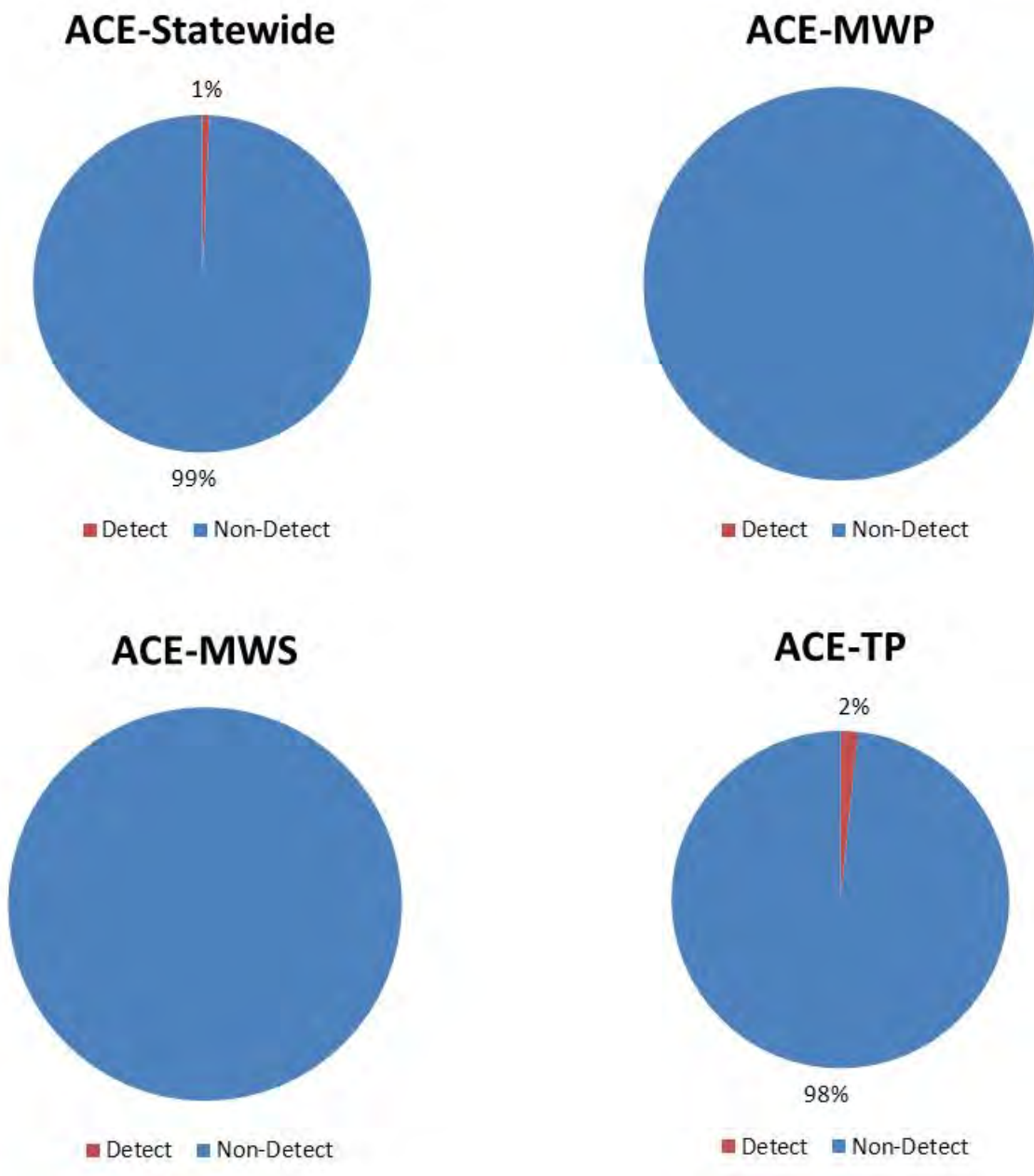


Figure 11. Estimated percentage of stream miles with detectable concentrations of acesulfame across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

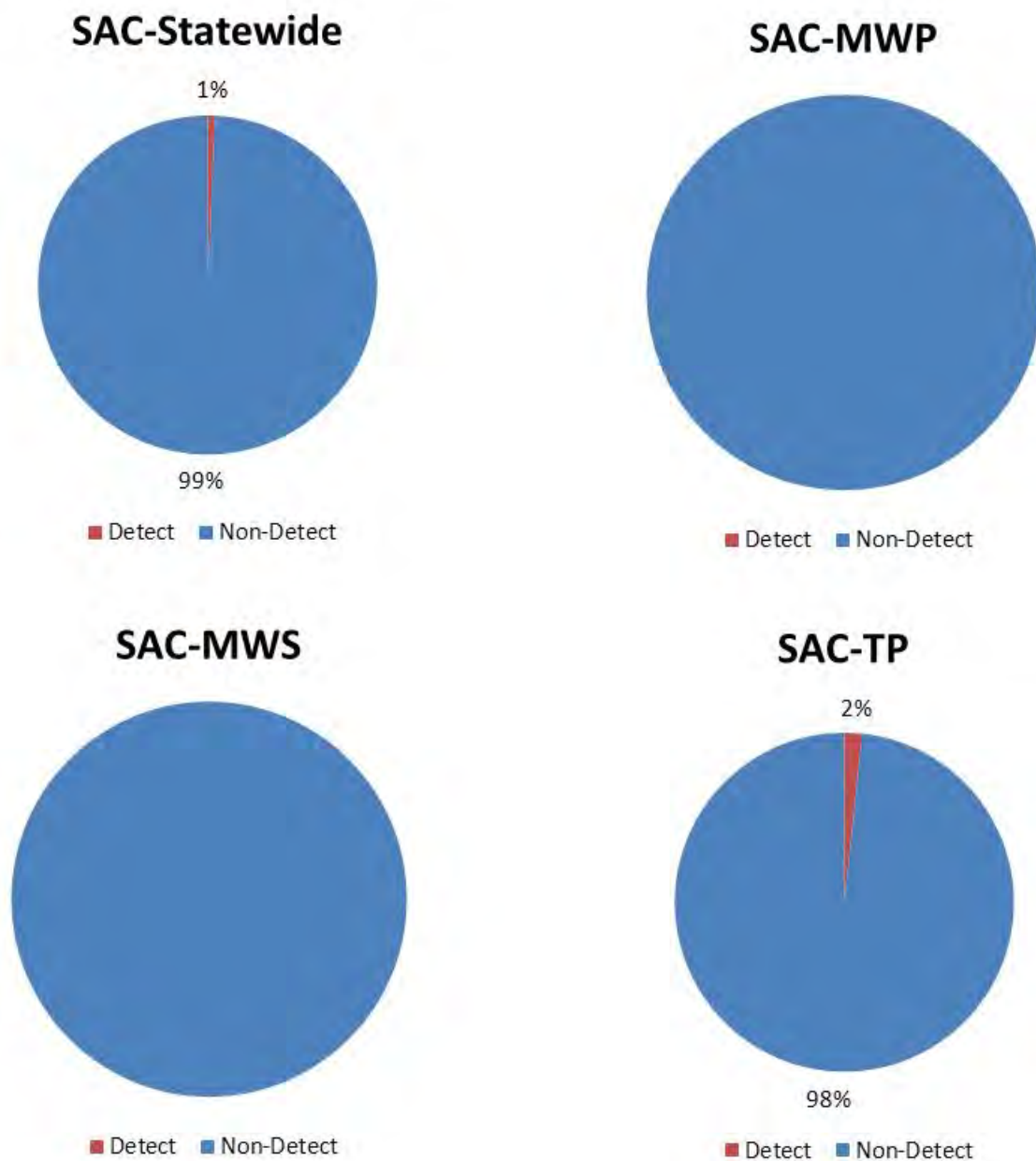


Figure 12. Estimated percentage of stream miles with detectable concentrations of saccharine across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

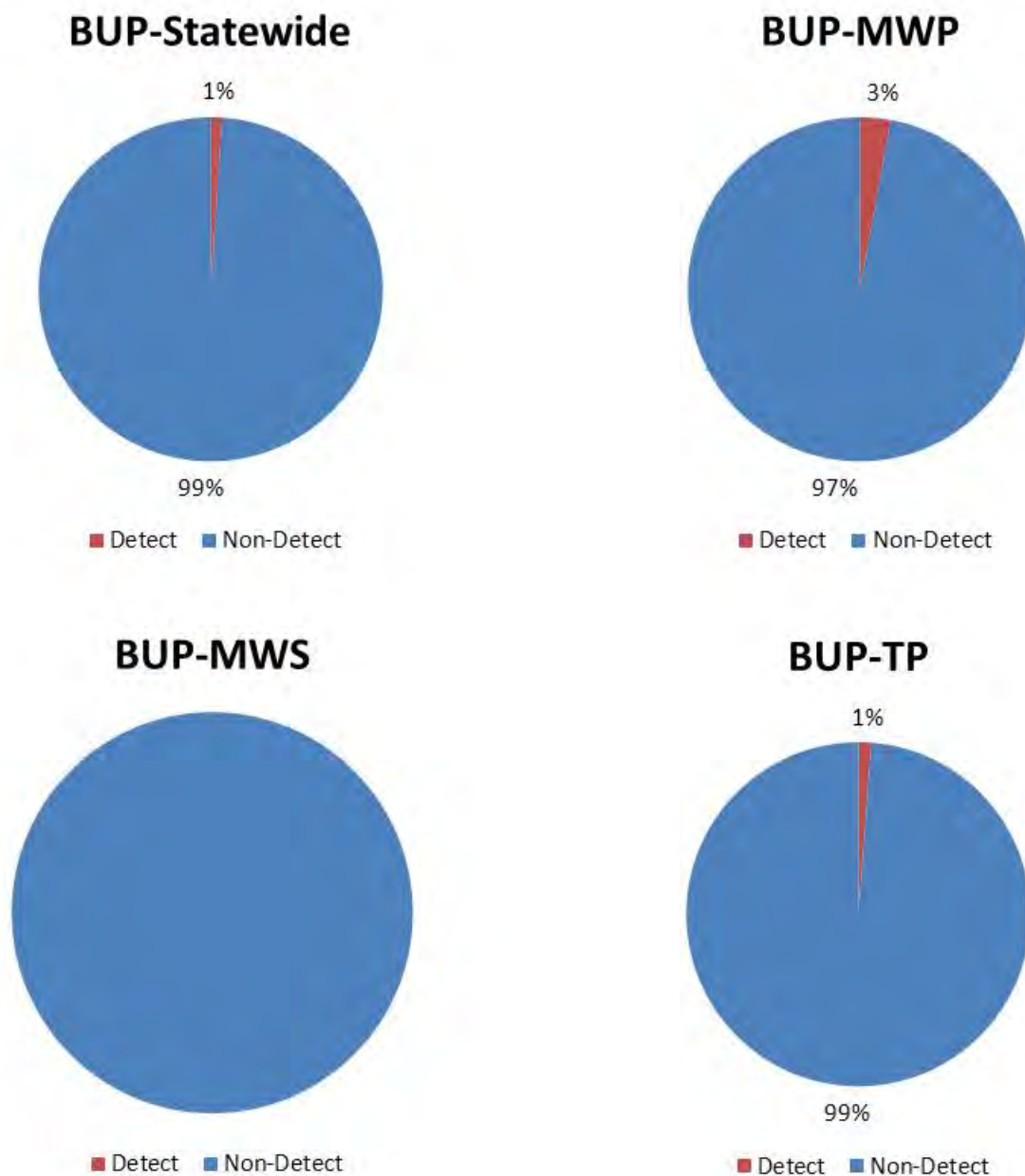


Figure 13. Estimated percentage of stream miles with detectable concentrations of bupropion across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

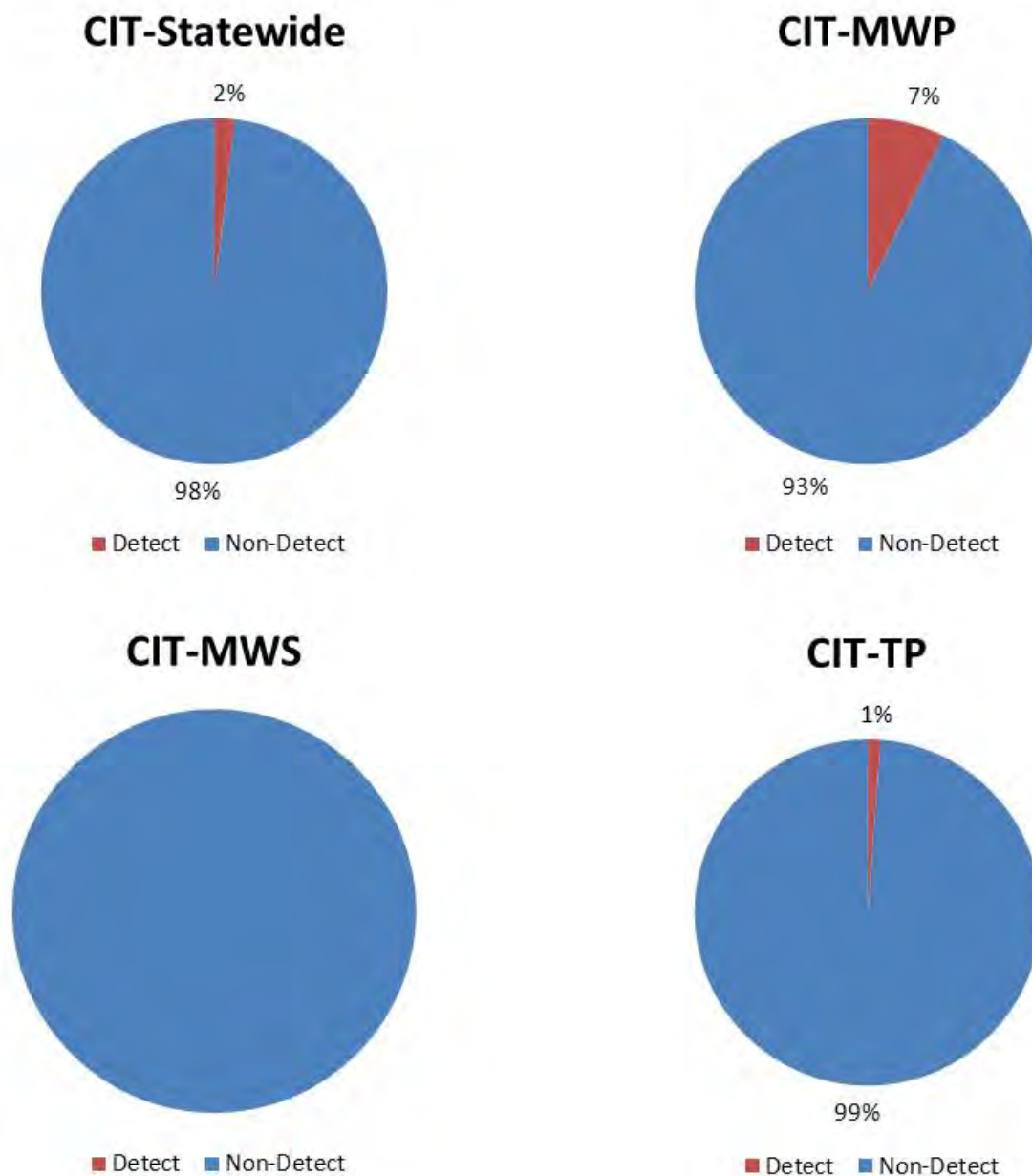


Figure 14. Estimated percentage of stream miles with detectable concentrations of citalopram across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

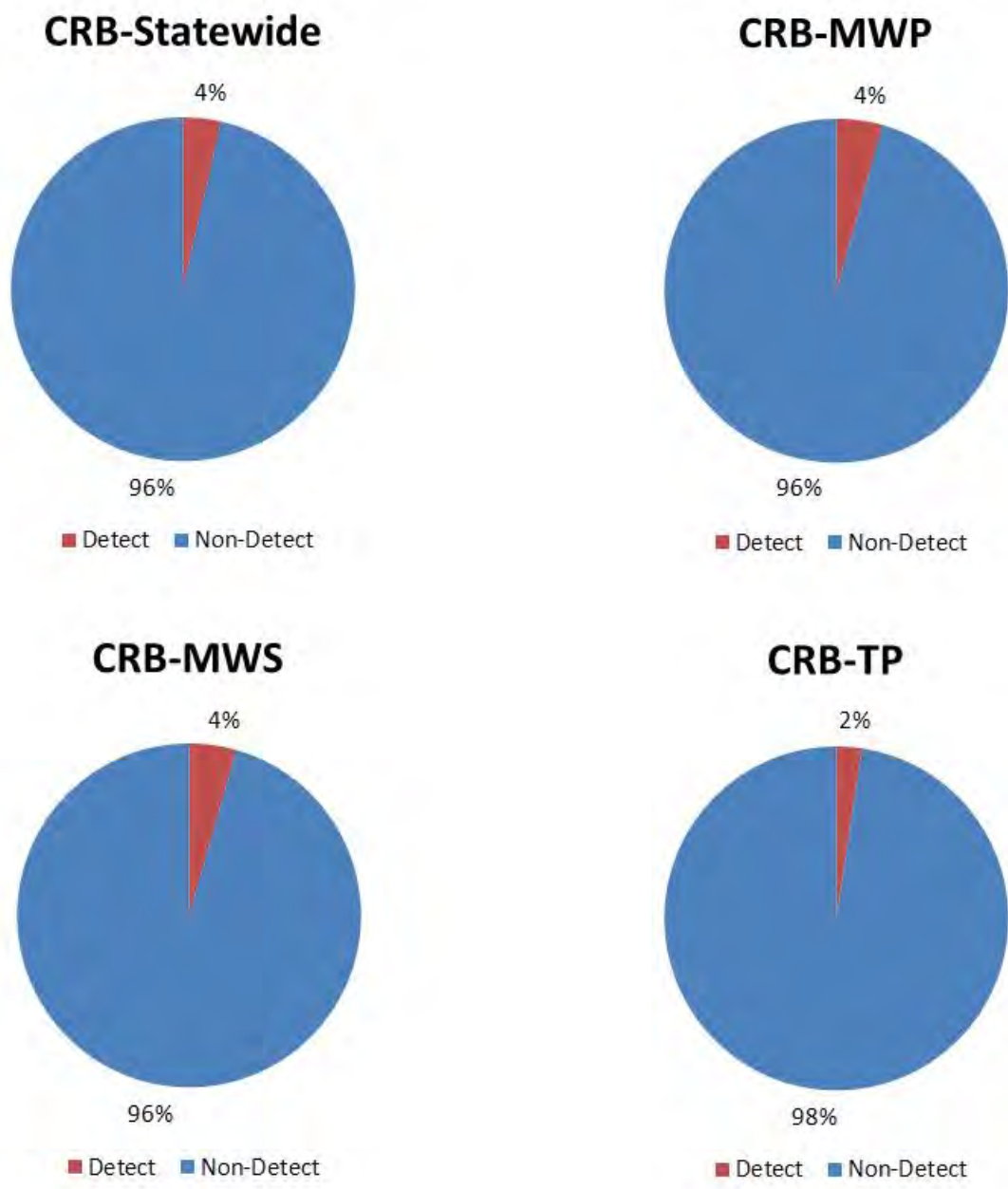


Figure 15. Estimated percentage of stream miles with detectable concentrations of carbamazepine across Minnesota (statewide) and within each of the state’s three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

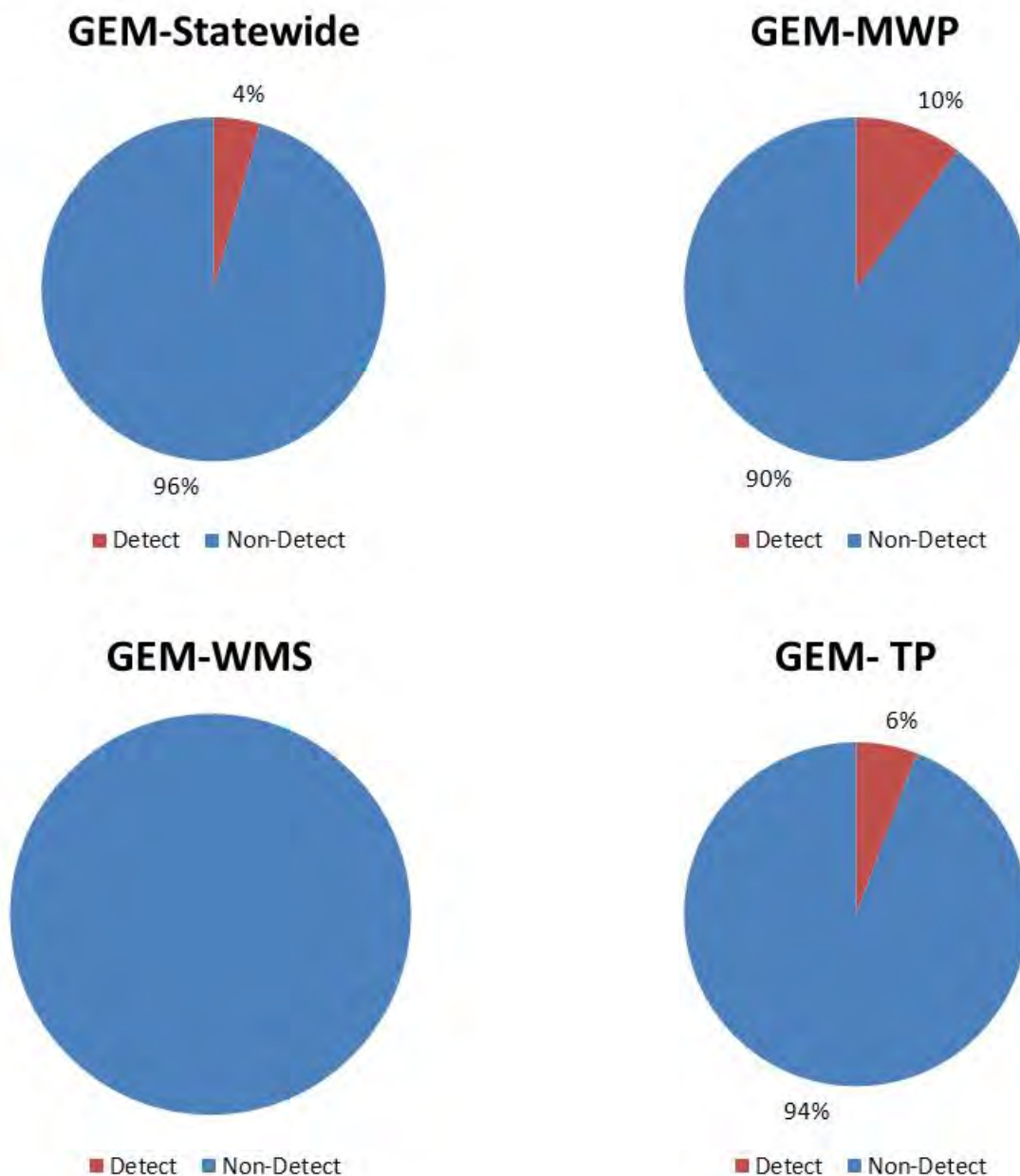


Figure 16. Estimated percentage of stream miles with detectable concentrations of gemfibrozil across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

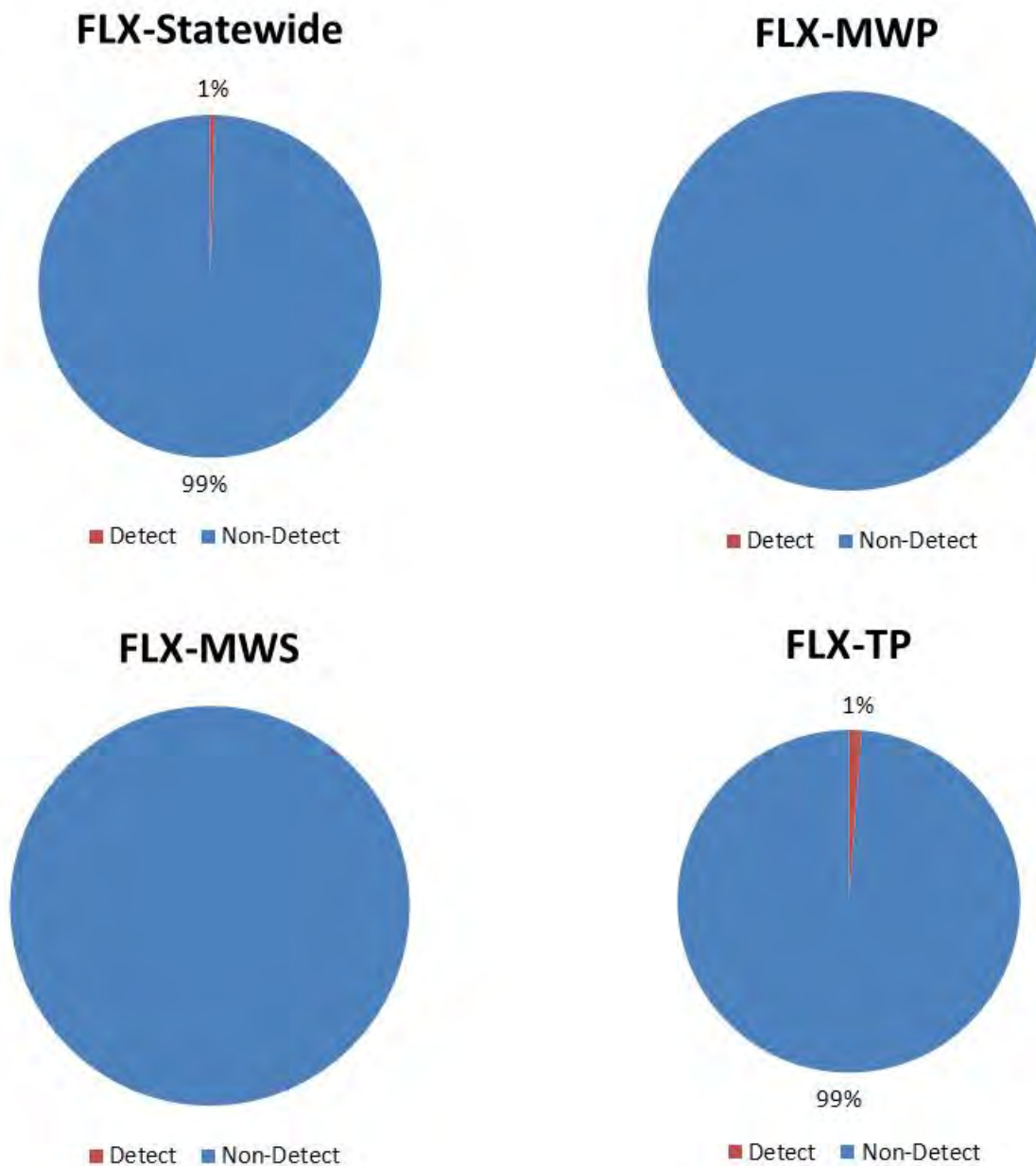


Figure 17. Estimated percentage of stream miles with detectable concentrations of fluoxetine across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

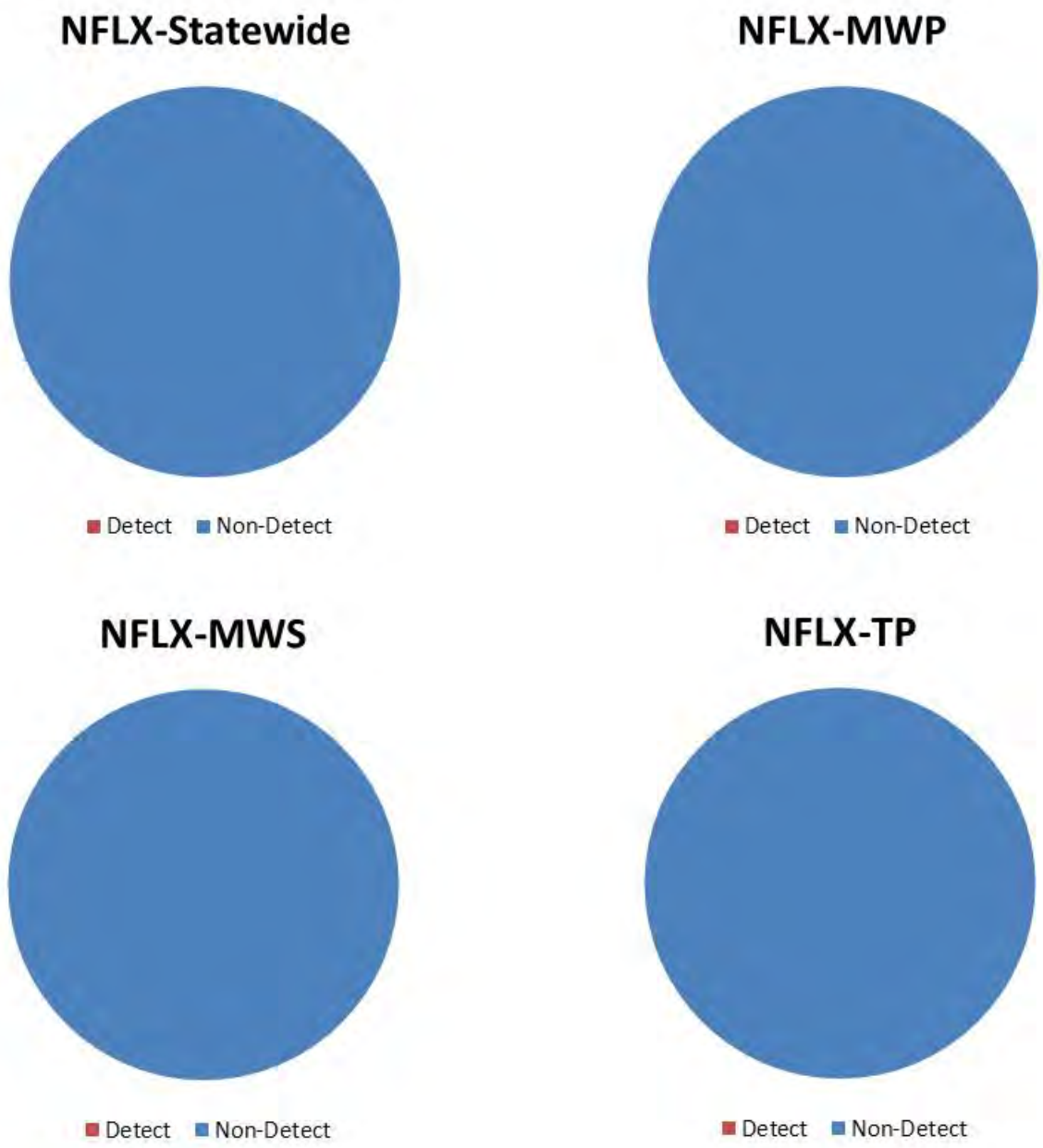
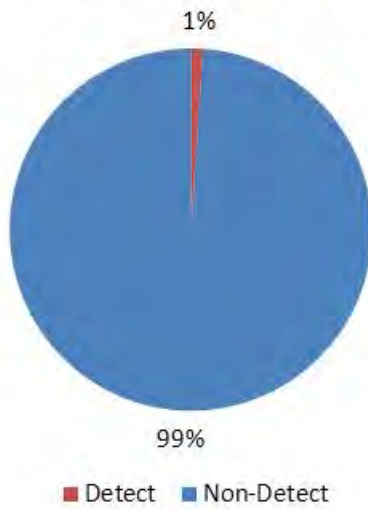


Figure 18. Estimated percentage of stream miles with detectable concentrations of norfluoxetine across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

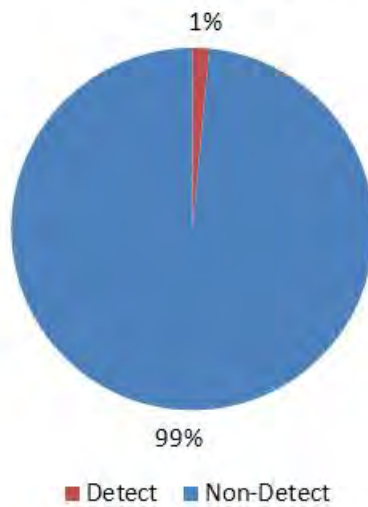
NSER-Statewide



NSER-MWP



NSER-MWS



NSER-TP

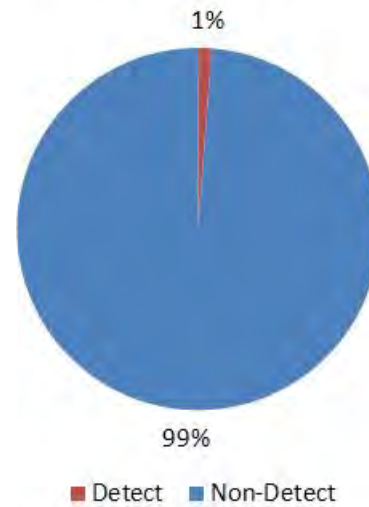


Figure 19. Estimated percentage of stream miles with detectable concentrations of norsesraline across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

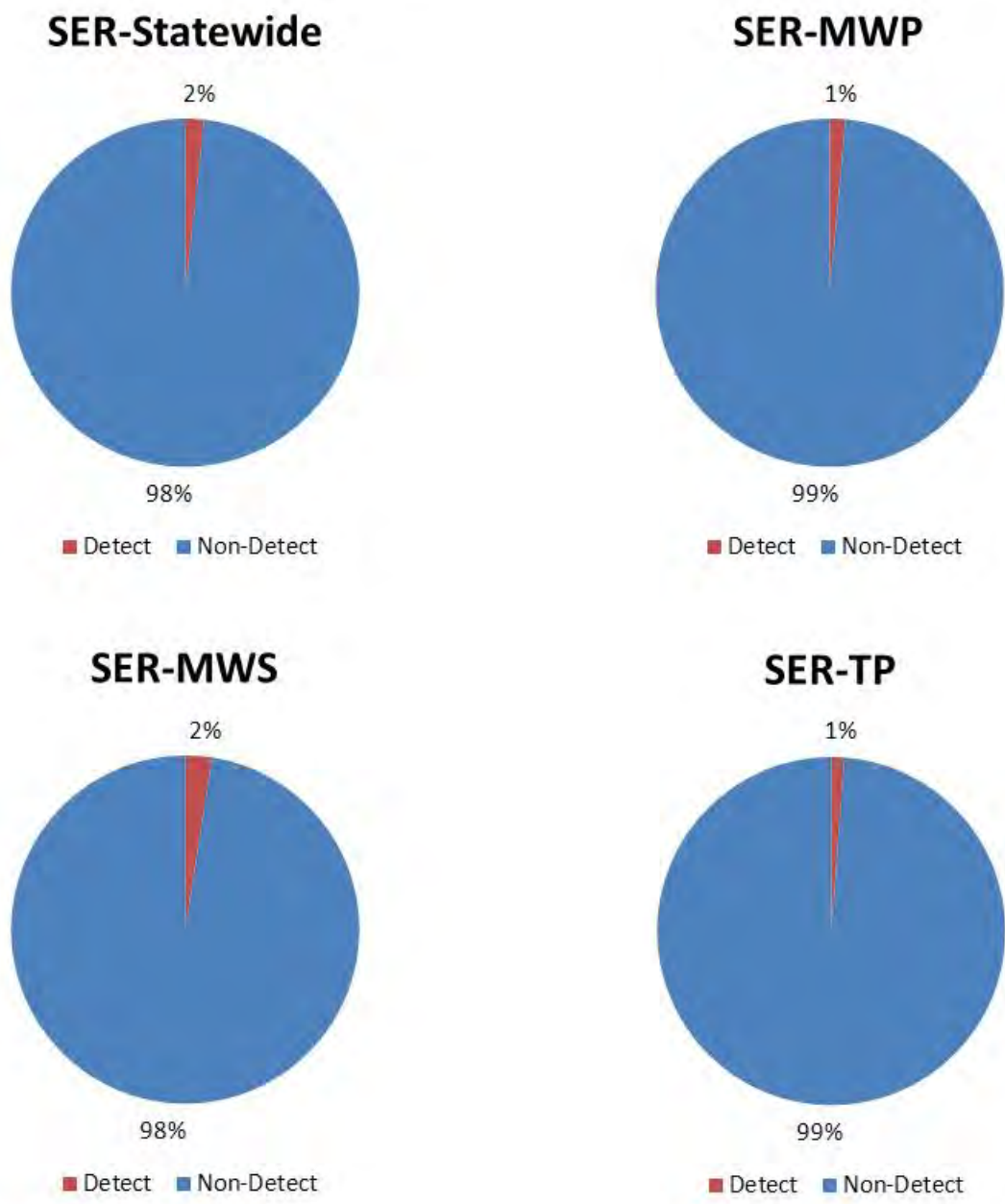


Figure 20. Estimated percentage of stream miles with detectable concentrations of sertraline across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

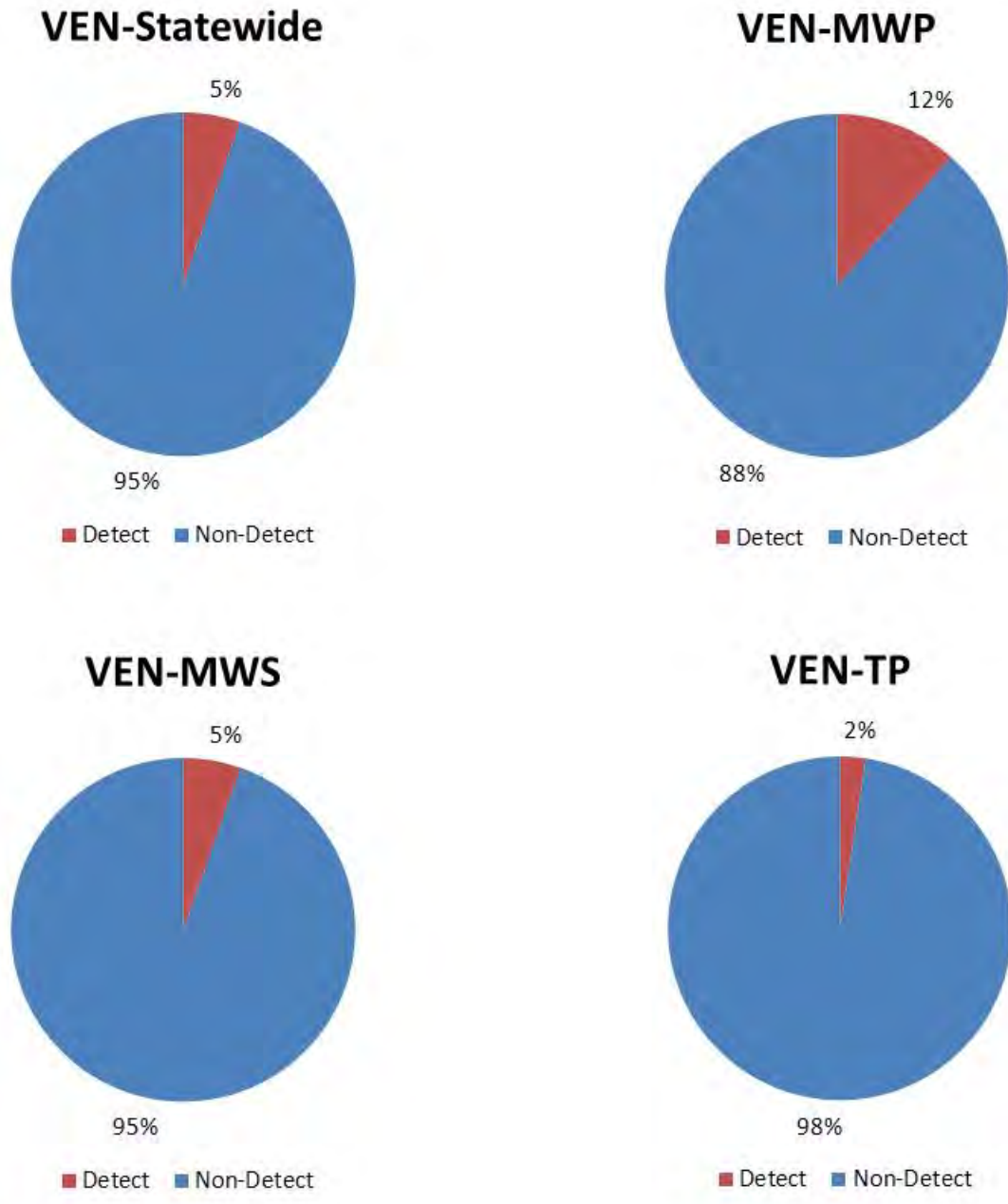


Figure 21. Estimated percentage of stream miles with detectable concentrations of venlafaxine across Minnesota (statewide) and within each of the state's three ecoregions (MWP, Mixed Wood Plains; MWS, Mixed Wood Shield; TP, Temperate Prairie).

Appendix A

Qualifier definitions

- The concentration of every target analyte in the method blank should be less than the report level.
- Samples above 10 times the method blank contamination are not qualified.
- A "B" qualifier is assigned to any sample target analyte in which the concentration is less than 10 times the concentration in the blank.
- A "B" qualifier means that the sample results may contain a bias related to method blank contamination.
- A "J" qualifier is assigned to values less than the report level; therefore this value is estimated.
- A "BJ" qualifier is assigned to values less than report level when there is a bias present due to method blank contamination.

Concentrations of analytes in water samples, laboratory blanks, spiked blanks, and duplicates. All concentrations are in ppt, or ng/L.

Sample ID	Benzo-triazole	Methyl benzo-triazole	Methyl paraben	Ethyl paraben	Propyl paraben	Butyl paraben	Benzyl paraben	Acesul fame	Saccharine	Bupropion	Citalopram	Carbamazepine	Gemfibrozil	Fluoxetine	Norfluoxetine	Norsertaline	Sertraline	Venlafaxine	
10G2090-01	17.68	492.74	14.46	B 0.59	BJ 2.16	B 0.26	BJ 0.16	J 490.4	B 40.24	B 0.47	J 1.77	5.39	B 12.02	0.71	J <1	<1	<1	3.09	
10G2090-02	<1	6.77	B 17.57	B 1.4	B 2.8	B 0.37	BJ <1	61.25	B <1	<1	<1	2.1	B <1	<1	<1	43.08	<1	<1	
10G2249-01	<1	5.35	B 52.15	1.78	B 4.38	B 0.45	BJ <1	119.3	B <1	<1	<1	5.39	B <1	<1	<1	<1	<1	1.38	
10G2249-02	<1	1.09	B 145.43	1.06	B 72.24	0.3	BJ <1	2.94	B <1	<1	<1	0.64	BJ <1	0.58	J <1	<1	<1	<1	
10G2249-03	<1	<1	113.17	0.93	BJ 17.05	B 0.16	BJ <1	3.92	B 17.07	B <1	<1	0.42	BJ <1	<1	<1	<1	3.63	<1	
10G2249-04	<1	<1	124.43	2.07	B 92.88	0.23	BJ <1	2.4	B 10.87	B <1	0.31	J 0.35	BJ <1	0.87	J <1	<1	1.73	<1	
10H0095-01	<1	4.07	B 53.54	0.91	BJ 3.36	B 0.2	BJ <1	260.22	B 34.26	B <1	<1	0.45	BJ <1	<1	<1	<1	<1	<1	
10H0095-02	<1	3.16	B 36.03	B 4.75	B 8.34	B 0.92	BJ <1	29.73	B <1	<1	<1	0.17	BJ <1	<1	<1	<1	<1	<1	
10H0095-03	<1	2.15	B 37.43	B 0.51	BJ 1.68	B 0.19	BJ <1	72.76	B 42.03	B <1	0.55	J 0.25	BJ <1	<1	<1	<1	<1	<1	
10H0098-01	132.95	375.86	18.74	B 0.62	BJ 2	B 0.14	BJ <1	981.06	B 35.17	B 3.02	3.17	23.41	9.27	<1	<1	<1	2.02	12.62	
10H0855-02	<1	2.63	B 71.06	0.76	BJ 3.09	0.4	BJ <1	5.73	B <1	<1	<1	0.19	BJ <1	<1	<1	<1	<1	<1	
10H0855-03	<1	1.73	B 24.63	B 0.57	BJ 7.76	0.26	BJ <1	3.8	B <1	<1	<1	0.23	BJ <1	<1	<1	<1	<1	<1	
10H1419-01	<1	3.29	B 43.03	0.8	BJ 2.69	0.32	BJ <1	8.23	B <1	<1	<1	0.17	BJ <1	<1	<1	<1	<1	<1	
10H1419-02	<1	1.45	B 19.48	B 0.73	BJ 1.99	0.36	BJ <1	23.86	B <1	<1	<1	0.45	BJ <1	<1	<1	<1	<1	<1	
10H1419-03	<1	2.05	B 45.6	0.69	BJ 2.59	0.29	BJ <1	19.09	B <1	<1	<1	0.22	BJ <1	<1	<1	<1	<1	<1	
10H1419-04	0.94	BJ 2.03	B 18.46	B 0.46	BJ 2.11	0.5	BJ <1	11.9	B <1	<1	<1	0.34	BJ <1	<1	<1	<1	<1	<1	
10H1419-05	1.94	B 4.88	B 22.55	B 0.99	BJ 3.45	0.98	BJ 0.16	J 78.24	B 12.08	B <1	<1	1.58	B <1	<1	<1	<1	<1	0.09	J
10H1419-07	1.38	B 1.95	B 25	B 0.6	BJ 2.78	0.6	BJ 0.15	J 14.56	B 8.66	B <1	<1	0.16	BJ <1	<1	<1	<1	<1	<1	
10H1419-08	2.92	B 5.14	B 31.95	B 1.32	B 2.36	0.42	BJ <1	99.59	B 18.62	B <1	<1	2.74	B <1	<1	<1	<1	<1	<1	
10H1419-09	<1	3.92	B 13.3	B 0.75	BJ 2.15	0.32	BJ <1	49.14	B 3.59	B <1	<1	0.47	BJ <1	0.12	J <1	<1	<1	<1	
10H1419-06	<1	1.51	B 9.79	B 0.39	BJ 1.27	B 0.26	BJ 0.22	J 8.6	B <1	<1	<1	0.15	BJ <1	<1	<1	<1	<1	<1	
10H1419-10	<1	2.02	B 36.3	0.87	BJ 0.8	BJ 0.23	BJ <1	33.12	B 25.29	B <1	<1	0.4	BJ <1	<1	<1	<1	0.4	J <1	
10H1456-01	<1	1.23	B 65.56	0.97	BJ 1.63	B 0.19	BJ <1	2	B <1	<1	<1	0.14	BJ <1	<1	<1	<1	<1	<1	
10H1456-02	<1	1.61	B 16.8	B 0.51	BJ 1.32	B 0.21	BJ <1	<1	<1	<1	<1	0.06	BJ <1	0.79	J <1	<1	<1	<1	
10H1456-03	<1	1.67	B 45.16	0.68	BJ 2.37	B 0.23	BJ <1	<1	<1	<1	<1	0.14	BJ <1	<1	<1	<1	<1	<1	
10H1456-04	<1	<1	53.66	0.79	BJ 2.29	B 0.27	BJ 0.17	J <1	<1	<1	<1	0.14	BJ <1	<1	<1	<1	<1	<1	
10H1456-05	<1	4.39	B 31.9	B 0.6	BJ 1.62	B 0.21	BJ <1	3.98	B <1	<1	<1	0.81	BJ <1	<1	<1	33.77	<1	<1	
10H1931-02	3.18	B 1082.7	10.96	B 0.39	BJ 0.97	BJ 0.16	BJ 0.1	J 86.65	B 27.04	B <1	<1	1.22	<1	<1	<1	<1	<1	<1	
10H1931-03	880.17	149.35	7.75	B 0.44	BJ 0.93	BJ 0.14	BJ <1	838.54	B 11.89	B 0.55	J 0.75	J 16.79	1.01	<1	<1	<1	<1	5.83	
10H1931-04	13.05	B 5.84	B 6.25	B 0.4	BJ 1	B 0.13	BJ 0.1	J 106.91	B 3.54	B <1	0.15	J 1.41	0.59	J <1	<1	<1	<1	0.38	J
10H1950-01	25.21	B 35.61	B 23.92	B 0.69	BJ 1.67	B 0.2	BJ 0.1	J 104.91	B 7.68	B <1	0.41	J 8.58	<1	<1	<1	<1	<1	0.41	J
10H1950-02	<1	4.84	B 32.49	0.73	BJ 1.35	B 0.17	BJ <1	10.75	B <1	<1	<1	0.03	BJ <1	<1	<1	<1	<1	<1	
10H1950-05	<1	1.67	B 18.7	B 0.63	BJ 1.26	B 0.18	BJ <1	23.86	B <1	<1	<1	0.09	BJ <1	<1	<1	<1	<1	<1	
10H1950-06	<1	4.54	B 34.1	0.52	BJ 1.03	B 0.14	BJ 0.09	J 11.72	B <1	<1	<1	0.66	BJ <1	<1	<1	<1	<1	<1	
10H2004-01	<1	918.12	39.13	1.14	1.2	B 0.12	BJ <1	51.72	B 17.42	B <1	<1	0.88	BJ <1	<1	<1	<1	<1	0.27	J
10H2004-02	<1	2.74	B 30.15	0.79	BJ 5.3	B 0.15	BJ <1	24.53	B <1	<1	<1	0.35	BJ <1	<1	<1	<1	<1	<1	
10H2004-06	<1	7.19	B 38.89	0.89	BJ 0.86	BJ 0.2	BJ <1	4.65	B <1	<1	<1	0.36	BJ <1	<1	<1	<1	<1	<1	
10G0996-01	1.97	B 0.75	BJ 25.72	B 1.75	B 8.6	B 0.88	BJ 0.21	J 31.87	B <1	<1	<1	0.2	BJ <1	0.03	BJ <1	<1	<1	0.07	J
10G0996-02	2.66	B 2.28	B 18.34	B 0.99	B 6.77	B 0.21	BJ 0.18	J 33.44	B <1	<1	<1	0.81	BJ <1	<1	<1	<1	<1	<1	
10G0996-04	<1	0.8	BJ 9.4	B 1.59	B 5.32	B 0.21	BJ 0.13	J 15.48	B 8.58	B <1	0.05	J 0.09	BJ <1	<1	<1	<1	<1	0.03	J
10G0996-07	<1	0.69	BJ 33.97	B 1.71	B 8.25	B 0.38	BJ <1	5.34	B <1	<1	<1	0.1	BJ <1	<1	<1	<1	<1	<1	
10G1000-01	<1	2.88	B 125.56	2.22	B 9.58	B 0.45	BJ <1	34.08	B <1	<1	<1	0.64	BJ <1	<1	<1	<1	<1	0.38	J

Sample ID	Benzo-triazole	Methyl benzo-triazole	Methyl paraben	Ethyl paraben	Propyl paraben	Butyl paraben	Benzyl paraben	Acesul fame	Sacch arine	Bupro pion	Citalo pram	Carbamaz-epine	Gemfi brozil	Fluox etine	Norfluox-etine	Norser traline	Sertra line	Venla faxine											
10I0922-02	<1	2.52	B	12.69	B	0.9	BJ	3.1	B	0.18	BJ	<1	1.46	B	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1					
10I1239-01	<1	1.21	B	35.69	B	0.46	BJ	1.39	B	0.15	BJ	<1	4.59	B	<1	<1	<1	0.02	BJ	<1	2.53	B	<1	<1	<1	<1			
10I1239-02	<1	1.68	B	32.92	B	0.4	BJ	1.2	B	0.12	BJ	<1	4.39	B	<1	<1	<1	0.18	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0130-01	<1	0.65	BJ	20.55	B	0.79	J	2.01	B	0.22	BJ	0.25	27.55	B	<1	<1	<1	0.72	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0132-07	<1	6.64	B	60.49	B	0.89	J	1.88	B	0.65	BJ	0.1	J	37.21	B	<1	<1	<1	0.23	BJ	<1	<1	<1	<1	<1	0.02	J		
10F0132-09	<1	<1		95.68		0.47	J	2.21	B	0.45	BJ	<1	<1	<1	<1	<1	<1	0.11	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0134-01	<1	2.59	B	190.56		0.82	J	2.08	B	0.3	BJ	0.21	J	43.39	B	<1	<1	<1	0.14	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0134-03	<1	1.8	B	374.06		1.05		3.3	B	0.47	BJ	0.42	J	5.16	B	<1	<1	<1	0.27	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0134-05	<1	0.34	BJ	109.55		2.42		3.55	B	0.53	BJ	<1	<1	<1	<1	<1	<1	0.15	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0135-01	<1	<1		357.72		1.6		5.26	B	0.39	BJ	<1	369.74	B	<1	<1	<1	0.27	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0135-02	<1	<1		436.26		3.61		7.02	B	0.61	BJ	<1	9.03	B	<1	<1	<1	0.2	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0135-03	<1	<1		268.71		1.24		3.06	B	0.35	BJ	0.31	J	23.09	B	<1	<1	<1	0.15	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0135-04	<1	<1		260.36		2.21		5.32	B	0.42	BJ	<1	14.32	B	<1	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1			
10F0132-01	9.53	B	41.26		30.94	B	4.52	B	6.09	B	2.02	BJ	<1	1382.87	B	38.01	B	2.47	2.13	7.88	B	9.06		<1	<1	<1	10.09		
10F0132-03	4.1	B	17.65	B	10.54	B	0.38	BJ	1.21	B	0.19	BJ	<1	802.7	B	6.77	B	0.82	J	4.22		0.86	J	0.28	J	<1	<1	<1	4.95
10F0132-05	<1	0.57	BJ	13.08	B	0.5	BJ	1.38	B	0.13	BJ	<1	746.37	B	12.71	B	<1	<1	<1	0.021	BJ	<1	<1	<1	<1	<1	<1		
10F0135-05	<1	3.11	B	142.11	B	15.73	B	18.92	B	3.11	BJ	<1	5.1	B	<1	<1	<1	0.03	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0135-06	<1	3.38	B	40.1	B	8.15	B	13.57	B	4.67		<1	32.89	B	<1	<1	<1	0.15	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0397-01	<1	<1		9.87	B	1.25	B	2.17	B	0.21	BJ	<1	13.98	B	15.23	B	<1	0.27	J	0.29	BJ	<1	<1	<1	<1	<1	<1	<1	
10F0397-02	<1	<1		16.51	B	0.29	BJ	0.93	BJ	0.09	BJ	<1	1.6	B	0.77	BJ	<1	<1	0.26	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0397-03	<1	<1		279.43		3.6	B	7.39	B	0.83	BJ	<1	3.03	B	<1	<1	<1	0.28	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0397-04	<1	<1		7.85	B	0.63	BJ	1.16	B	0.14	BJ	<1	4.73	B	5.74	B	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0502-04	<1	<1		103.49	B	5.2	B	14.68	B	5.16		<1	18.32	B	<1	<1	<1	0.13	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0397-05	<1	3.81	B	124.39	B	1.47	B	2.67	B	0.56	BJ	0.08	J	10.36	B	<1	<1	<1	0.07	BJ	<1	<1	<1	<1	<1	<1	<1		
10F0397-06	<1	2.74	B	110.82	B	2.59	B	4.03	B	0.34	BJ	<1	100.14	B	<1	<1	<1	0.89	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0502-01	<1	<1		292.01		1.66	B	3.05	B	0.26	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1		
10F0502-02	<1	<1		311.53		1.57	B	4.15	B	0.22	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1		
10F0502-03	<1	11.84	B	183.43	B	2.03	B	3.75	B	0.41	BJ	<1	4.06	B	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1		
10F0882-01	<1	6.34	B	83.89	B	1.45	B	2.92	B	0.37	BJ	<1	155.07	B	<1	<1	<1	0.59	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0882-02	<1	4.53	B	114.96	B	3.36	B	6.56	B	0.6	BJ	<1	8.76	B	<1	<1	<1	0.19	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0882-03	<1	5.02	B	131.31	B	4.22	B	7.97	B	0.54	BJ	<1	67.06	B	<1	<1	<1	0.32	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0930-01	<1	4.38	B	168.52	B	3.93	B	6.69	B	0.49	BJ	<1	<1	<1	<1	<1	<1	0.17	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0930-02	<1	4.4	B	110.45	B	2.63	B	4.96	B	0.47	BJ	<1	<1	<1	<1	<1	<1	0.13	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0930-03	<1	<1		71.08	B	3.73	B	6.93	B	0.62	BJ	<1	<1	<1	<1	<1	<1	0.23	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0930-07	<1	4.57	B	143.14	B	2.37	B	4.78	B	0.72	BJ	<1	<1	<1	0.46	J	<1	0.52	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0882-04	<1	<1		192.12	B	1.6	B	3.09	B	0.58	BJ	<1	<1	<1	<1	<1	<1	0.38	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0882-05	<1	4.6	B	174.38	B	1.78	B	3.48	B	0.28	BJ	<1	3.36	B	<1	<1	<1	0.59	BJ	<1	<1	<1	<1	<1	<1	0.16	J		
10F0903-04	<1	<1		103.6	B	2.61	B	3.81	B	0.38	BJ	<1	<1	<1	<1	<1	<1	0.56	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0903-06	<1	<1		252.42		1.54	B	4.23	B	0.23	BJ	<1	<1	<1	<1	<1	<1	0.87	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10F0903-05	<1	11.31	B	65.2	B	1.8	B	3.83	B	0.66	BJ	<1	91.54	B	<1	<1	<1	0.69	J	34.1		<1	<1	<1	<1	<1	1.62		
10G0048-02	<1	3.06	B	136.81	B	1.16	B	2.33	B	0.43	BJ	<1	3.99	B	<1	<1	<1	0.16	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10G0048-01	<1	<1		398.75		1.82	B	2.76	B	0.4	BJ	<1	<1	<1	<1	<1	<1	0.18	BJ	<1	<1	<1	<1	<1	<1	<1	<1		
10G0154-01	<1	3.97	B	122.41	B	2.01	B	4.09	B	0.46	BJ	<1	1.78	B	<1	<1	<1	0.26	BJ	<1	<1	<1	<1	<1	<1	<1	<1		

Sample ID	Benzo-triazole	Methyl benzo-triazole	Methyl paraben	Ethyl paraben	Propyl paraben	Butyl paraben	Benzyl paraben	Acesul fame	Sacch arine	Bupro pion	Citalo pram	Carbamaz-epine	Gemfi brozil	Fluox etine	Norfluox-etine	Norser traline	Sertra line	Venla faxine																		
10G0154-02	<1	5.74	B	235.65	B	2.25	B	4.14	B	0.49	BJ	<1	6.1	B	<1	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1		
10G0048-03	7.89	B	13.35	B	36.29	B	0.48	BJ	1.08		0.22	BJ	<1	297.3	B	<1	<1	1.21	B	1.84	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1		
10G0048-04	7.16	B	17.44	B	33.32	B	0.5	BJ	0.86	BJ	0.13	BJ	<1	402.32	B	<1	<1	1.71	B	2.48	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0154-03	<1		4	B	92.15	B	<1		1.59		<1		<1	5.12	B	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0154-04	<1		5.79	B	69.87	B	<1		1.28		0.08	BJ	<1	10.62	B	<1	<1	0.16	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0154-05	<1		4.65	B	416.12		<1		1.73		<1		<1	<1	<1	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0463-01	<1		3.38	B	60.42	B	0.76	BJ	1.51		<1		<1	4.72	B	<1	<1	0.26	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0463-02	7.58	B	16.57	B	75.19	B	0.86	BJ	5.78		0.37	BJ	<1	306.62	B	<1	0.54	J	<1	3.63	B	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	1.79	<1	<1	
10G0463-03	<1		3.54	B	92.86	B	1.32	B	4.94		0.8	BJ	<1	9.36	B	<1	<1	0.36	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0465-01	<1		2.8	B	366.02		1.32	B	83.28		0.26	BJ	<1	<1		<1	<1	0.16	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0465-02	<1		3.42	B	119.01		<1		6.55		<1		<1	<1		<1	<1	<1		<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	
10G0465-03	<1		4.03	B	88.46	B	0.7	BJ	2.07		0.12	BJ	<1	74.05	B	<1	<1	0.37	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0465-04	<1		0.9	BJ	65.22	B	0.93	BJ	12.71		0.14	BJ	<1	14.39	B	<1	<1	0.35	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0510-01	<1		19.96	B	70.88	B	<1		0.99		0.1	BJ	<1	312.56	B	13.18	B	<1	0.2	J	1.28	B	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	0.16	J	<1	<1
10G0510-02	<1		<1		184.89		1.66	B	5.56		0.37	BJ	<1	4	B	<1	<1	0.99	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0510-03	<1		<1		61.49	B	0.7	BJ	2.07		0.22	BJ	<1	<1		<1	<1	0.5	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0510-04	<1		<1		123.11		0.8	BJ	1.37		<1		<1	7.73	B	<1	<1	0.25	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0996-03	<1		0.7	BJ	10.84	B	0.92	BJ	1.52		0.18	BJ	<1	4.52	B	<1	<1	0.26	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	0.28	J	<1	<1
10G0996-05	<1		0.6	BJ	11.14	B	0.66	BJ	1.14		0.25	BJ	<1	5.14	B	<1	<1	0.35	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G0996-06	<1		1.05	B	47.92	B	<1		1.06		0.1	BJ	<1	35.83	B	<1	<1	1.52	B	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
10G1026-01	<1		2.36	B	1000.79		0.73	BJ	597.99		0.2	BJ	0.07	J	11.97	B	<1	<1	0.35	BJ	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1

Quality assurance data

Sample ID	Benzo- triazole	Methyl benzo- triazole	Methyl paraben	Ethyl paraben	Propyl paraben	Butyl paraben	Benzyl paraben	Acesul fame	Sacch arine	Bupro pion	Citalo pram	Carbamaz- epine	Gemfi brozil	Fluox etine	Norfluox- etine	Norser traline	Sertra line	Venlafaxine
20100810 Blnk	<1	5.94	4.67	2.41	4.14	0.25	<1	384.48	33.91	<1	<1	1.04	<1	<1	<1	<1	<1	<1
20100810 Blnk Spk	59.36	52.85	B 61.03	79.98	119.75	49.02	35.14	458.38	B 72.14	B 32.66	51.13	53.27	61.49	51.21	47.11	49.38	53.73	57.89
20100810 Blnk Spk Dup	61.32	53.3	B 61.37	83.7	114.38	50.41	26.85	463.28	B 73.16	B 33.77	51.04	54.64	51.16	53.28	41.72	66.59	52.45	56.43
10G2090-02 spk	55.79	54.4	B 70.26	89.12	116.68	50.95	26.06	118.89	B 59.95	B 33.95	51.85	53.2	57.93	53.44	46.55	57.95	53.22	56.49
10G2090-02 spk dup	59.32	55.92	B 69.98	90.29	115.53	51.9	24.87	120.67	B 53.17	B 33.71	50.53	54.22	58.76	52.32	43.8	67.2	52.25	58.8
20100824 Blnk	7.33	3.89	3.7	0.94	<1	1.13	<1	337.57	18.43	<1	<1	1.19	<1	<1	<1	<1	<1	<1
20100824 Blnk Spk	60.75	B 56.06	<1	<1	<1	<1	<1	<1	<1	35.61	53.62	56.75	<1	51.46	39.77	46.64	57.91	58.14
20100824 Blnk Spk Dup	59.41	B 57.48	60.27	80.21	100.06	52.66	33.65	369.41	B 71.54	B 35.45	53.8	56.56	61.2	54.92	49.9	52.25	51.3	60.18
10H0855-02 spk	52.48	B 50.87	139.8	104.91	159.68	53.25	23.66	59.93	B 62.43	B 36.65	52.09	56.32	57.26	56.49	48.16	59.45	54.75	59.24
10H0855-02 spk dup	61.92	B 51.38	131.51	106.65	176.5	52.57	23.75	63.53	B 62.56	B 36.19	53.68	55.98	61.48	54.82	52.64	42.59	54.49	60.39
20100827 Blnk	6.71	3.49	3.21	0.63	1.38	0.72	<1	313.18	18.9	<1	<1	1.15	<1	<1	<1	<1	<1	<1
20100827 Blnk Spk	58	B 54.68	57.85	80.88	104.92	50.29	32.88	354.36	B 71.7	B 35.35	51.19	55.75	56.95	52.15	48.46	53.03	54.89	59.61
20100827 Blnk Spk dup	57.6	B 55.12	59.8	81.74	103.87	51.91	32.08	346.97	B 69.49	B 35.07	53.16	55.34	55.03	56.74	49.29	63.45	54.22	60.04
10H1456-05 Dup	<1	5.82	B 30.12	B 0.55	BJ 1.59	B 0.18	BJ <1	3.88	B <1	<1	<1	0.21	BJ <1	<1	<1	<1	<1	<1
10H1419-06 Spk	52.87	B 51.7	69.59	88	106.64	51.8	36.74	69.46	B 54.91	B 34.83	53.33	54.13	52.25	54.16	47.86	57.24	51.95	57.93
10H1419-06 Spk Dup	51.03	B 53.5	65.99	85.84	107.57	50.66	32.67	66.56	B 55.52	B 34.35	52.28	53.29	59.9	53.8	48.89	60.08	57.3	57.7
20100902 Blnk	6.93	5.9	2.71	0.76	1.76	0.73	<1	283.27	17.39	<1	<1	0.84	<1	0.09	<1	<1	0.07	<1
20100902 Blnk Spk	55.65	B 55.97	B 60	83.31	109.12	52.55	30.17	391.53	B 72.31	B 35.11	53.91	56.71	58.53	53.42	50.87	58.74	54.33	60.5
20100902 Blnk Spk Dup	57.27	B 56.49	B 60.33	82.91	108.07	51.15	29.08	377.01	B 73.94	B 34.58	52.06	57.69	57.28	54.53	45.15	47.52	56.53	58.36
10H1931-03 spk	991.24	253.61	63.74	75.84	87.96	50.7	38.38	932.95	B 63.52	B 35.12	53.28	70.85	55.4	54.98	49.5	62.87	55.06	65.74
10H2004-01 Dup	<1	903.31	27.24	0.62	BJ 1.23	B 0.3	BJ <1	51.74	B 14.42	B <1	<1	0.94	BJ <1	6.18	<1	<1	<1	0.24
20100728 Blnk	10	7.66	6.56	1.85	20.18	3.43	<1	327.01	23.54	<1	<1	0.88	<1	0.06	<1	<1	<1	<1
20100728 Blnk Spk	61.4	B 50.74	B 87.07	72.77	129.59	B 52.77	39.4	458.14	B 66.4	B 31.54	50.5	51.43	54.66	57.49	46.51	48.11	50.37	53.12
20100728 Blnk Spk Dup	59.94	B 51.69	B 75.63	72.69	131.62	B 54.19	41.35	385.47	B 66.72	B 31.68	49.28	51.54	60.71	57.75	47.99	46.16	52.13	52.59
10G0996-04 Spk	50.59	B 47.66	B 79.04	77.26	115.27	B 51	36.71	68.07	B 49.72	B 31.18	49.27	49.48	55.11	55.29	46.29	53.68	50.26	52.21
10G0996-04 Spk Dup	52.21	B 48.48	B 63.17	B 72.4	98.48	B 50.28	38.8	68.68	B 57.84	B 31.02	48.47	50.12	62.43	54.89	47.75	50.61	52.3	53.54
10G1026-04 Dup	<1	29.97	B 261.83	5.03	B 29.97	B 1.96	B 0.47	J 5640.2	403.74	<1	<1	2.02	134.35	<1	<1	<1	<1	0.05
20100803 Blnk	8.76	3.9	10.23	6.71	11.21	0.86	<1	404.67	28.11	<1	<1	1.36	<1	<1	<1	<1	<1	<1
20100803 Blnk Spk	56.42	B 51.04	82.23	B 86.26	150.27	49.79	46.82	406.47	B 59.75	B 31.33	49.98	55.04	<1	57.35	46.43	46	50.67	51.91
20100803 Blnk Spk Dup	63.24	B 50.79	96.38	B 71.82	129.26	50.77	52.4	471.13	B 68.27	B 31.95	50.92	52.38	58.22	55.6	44.55	47.89	52.31	51.87
10G1647-01 Spk	700.01	572.97	65.16	B 81.42	113.84	47.84	41.14	1698.6	B 69.1	B 35.7	60.21	65.41	59.64	52.48	44.07	56.86	50.82	89.11
10G1647-01 Spk Dup	690.92	578.95	92.79	B 79.37	125.76	49.95	39.55	1738.5	B 60.44	B 35.03	61.22	63.78	63.82	55.43	50.22	46.65	52.56	81.74
20100817 Blnk	8.62	5.58	10.9	2.69	4.77	1.59	<1	379.97	26.68	<1	<1	1.53	<1	<1	<1	<1	<1	<1
20100817 Blnk Spk	59.66	B 57.47	59.57	B 81.98	125.86	51.62	39.83	407.53	B 71.7	B 33.15	51.94	55.47	47.44	57.38	49.12	47.28	53.15	54.99

Sample ID	Benzo-triazole		Methyl benzo-triazole		Methyl paraben		Ethyl paraben		Propyl paraben		Butyl paraben		Benzyl paraben		Acesul fame		Sacch arine		Bupro pion		Citalo pram		Carbamaz-epine		Gemfi brozil		Fluox etine		Norfluox-etine		Norser traline		Sertra line		Venlafaxine
20100817 Blnk Spk Dup	60.12	B	53.87	B	62.93	B	83.51		122.1		51.75		40.86		453.79	B	74.81	B	34.3		52.2		51.75		56.12		56.64		48.2		53.06		54.36		54.8
10H0855-02 Spk	56.54	B	51.22	B	102.17	B	90.18		124.26		51.91		25.83		102	B	80.38	B	33.83		51.06		52.04		57.52		53.98		48.1		47.63		54.24		54.55
10H0855-02 Spk Dup	56.6	B	51.82	B	102.88	B	90.07		131.34		51.42		26		99.48	B	75.99	B	33.57		51.4		52.23		59.9		53.31		49		50.08		51.67		55.39
20100908 Blnk	5.7		4.01		2.88		0.79		0.81		<1		2.77		403.75		18.61		<1		<1		0.88		<1		0.64		0.46		<1		1.08		<1
20100908 Blnk Spk	55.77	B	58.13		56.61		72.71		101.32		54.3		26.88	B	444.23	B	66.23	B	34.53		52.93		55.25		52.28		47.95		45.35		43.88		53.27		65.23
20100908 Blnk Spk Dup	52.82	B	55.18		56.71		77.12		109.59		53.87		31.71	B	448.68	B	68.01	B	35.02		53.38		56.53		54.67		46.27		47.98		64.52		52.29		64.07
10H1931-01 spk	180.75		380.83		60.3		73.75		91.97		51.76		27.44	B	392.64	B	60.75	B	35.1		52.73		59.98		52.59		47.58		44.26		41.92		48.45		64.5
10H1931-01 dup spk	189.71		662.69		63.64		74.32		97.2		55.03		24.78	B	407.16	B	70.12	B	35.41		53.04		65.1		52.39		48.97		49.06		52.37		50.58		62.65
20100921 Blnk	6.02		3.46		4.74		1.03		1.35		0.33		<1		345.37		16.89		<1		<1		0.88		<1		<1		<1		<1		<1		<1
20100921 Blnk Spk	55.13	B	57.46		57.46		72.44		96.22		53.36		30.92		403.05	B	66.4	B	34.77		54.26		57.38		54.12		47.69		45.88		46.84		48.89		62.86
20100921 Blnk Spk Dup	58.34	B	55.81		56.36		70.19		84.79		53.38		36.89		390.39	B	69.52	B	34.89		54.01		56.9		50.58		48.78		45.97		49.07		50.99		63.55
10I0922-01 Spk	55.22	B	55.11		163.51		87.06		152.88		57.78		16.96		78.05	B	59.92	B	35.28		50.61		56.96		58.68		49		54.55		<1		37.15		63.49
10I0922-01 Dup Spk	51.09	B	54.93		216.6		85.73		152.8		54.57		15.15		73.76	B	59.18	B	36.53		49.85		56.69		57.13		46.68		49.07		<1		41		64.41
20101005 Blnk	5.7		4.09		4.25		0.47		0.94		0.43		<1		281.65		12.73		<1		<1		1.06		<1		0.31		<1		<1		<1		<1
20101005 Blnk Spk	53.9	B	54.61		58.64		71.54		85.12		55.25		27.34		363.49	B	70.59	B	36.44		52.77		57.97		59.32		46.7		44.6		45.69		50.96		65.94
20101005 Blnk Spk Dup	57.99		57.89		57.22		75.1		108.16		55		24.82		350.11	B	65.29	B	37.63		54.12		56.8		60.99		45.64		43.63		37.81		46.8		64.14
10I1239-01 Spk	47.68	B	56.18		83.71		91.67		134.85		56.03		15.17		84.35	B	55.71	B	36.01		52.36		58.08		64.06		47.28		40.02		51.64		50.56		65.65
10I1239-02 Dup	<1		1.71	B	35.26	B	0.6	BJ	1.23	B	<1		<1		4.44	B	<1		<1		<1		0.36	BJ	<1		<1		<1		<1		<1		<1
20100618 Blnk	7.94		2.72		76.51		<1		1.86		0.48		<1		462.32		57.17		<1		<1		1.15		<1		<1		<1		<1		<1		<1
20100618 Blnk Spk	52.66	B	55.98		148.09		46.11		55.31		53.47		57.4		488.34	B	127.31	B	32.46		50.91		50.95		53.71		52.98		45.44		56.75		48.51		53.99
20100618 Blnk Spk Dup	49.54	B	52.59		131.17		47.95		56.9		53.43		58.43		505.09	B	185.98	B	31.13		51.24		50.29		58.11		52.97		47.15		61.73		47.74		53.18
10F0132-07 Dup	<1		5.41	B	89.6		1.13		1.78	B	0.41	BJ	<1		36.23	B	<1		<1		<1		0.21	BJ	<1		<1		<1		<1		<1		<1
10F0134-05 Spk	48.97	B	47.97		197.96		40.58		43.8		52.99		71.89		55.6	B	<1		29.95		49.91		49.08		53.85		53.18		47.44		56.9		51.14		53.28
20100622 Blnk	8.4		3.23		18.51		7.64		9.42		0.44		<1		414.31		36.57		<1		<1		1.5		<1		<1		<1		<1		<1		<1
20100622 Blnk Spk	53.2	B	52.83		72.83	B	73.53	B	86.9	B	53.3		45.25		433.65	B	77.85	B	31.1		50.92		50.89		53.28		52.05		45.61		52.66		50.47		53.78
20100622 Blnk Spk Dup	51.49	B	50.85		61.02	B	67.6	B	78.98	B	52.79		39.17		431.05	B	93.82	B	29.54		48.66		51.23		53.79		50.66		43.64		58.44		49.2		53.93
10F0135-05 Dup	<1		2.95	B	51.35	B	2.98	B	4.59	B	0.63	BJ	<1		6.4	B	<1		<1		<1		0.26	BJ	<1		<1		<1		<1		<1		<1
10F0397-04 Spk	53.17	B	52.89		327.09		80.3		119.94		51.48		19.8		60.34	B	49.25	B	30.5		48.75		50.31		62.87		52.25		51.2		<1		49.09		55.16
20100629 Blnk	6.61		4.94		23.04		6.91		8.46		0.48		<1		431.77		32.15		<1		<1		0.88		<1		<1		<1		<1		<1		<1
20100629 Blnk Spk	52.4	B	52.83		153.35	B	122.67		134.2		49.92		48.07		434.81	B	87.98	B	30.72		47.51		53.54		<1		47.66		48.03		50.71		48.61		51.64
20100629 Blnk Spk Dup	52.87	B	52.8		103.04	B	85.66		93.27		51.25		47.69		440.83	B	80.77	B	30.69		45.08		53.15		<1		47.89		47.21		56.86		49.4		52.07
10F0882-01 spk	49.42	B	53.67		132.47	B	69.46		92.43		47.96		28.17		204.31	B	70.87	B	28.66		46.36		48.98		51.84		46.36		45.31		48.48		49.98		49.51
10F0882-01spk dup	48.07	B	52.12		114.06	B	78.3		95.61		50.53		27.24		200.75	B	64.43	B	28.29		47.75		50.09		49.97		48.15		44.88		52.43		50.22		49
10F0930-03 dup	<1		4.08	B	82.36	B	3.78	B	6.25	B	0.68	BJ	<1		<1		<1		<1		<1		0.36	BJ	<1		<1		<1		<1		<1		<1
20100706 Blnk	16.84		6.23		24.86		5.61		3.9		1.05		<1		392.98		38.56		<1		<1		2		<1		<1		<1		<1		<1		<1
20100706 Blnk Spk	56.13	B	53.43	B	70.08	B	63.22		66.55		47.05		33.04		441.34	B	74.52	B	31.8		50.12		49.7		46.47		50.82		53.34		58.46		47.65		52.14

Sample ID	Benzo-triazole		Methyl benzo-triazole		Methyl paraben		Ethyl paraben		Propyl paraben		Butyl paraben		Benzyl paraben		Acesulfame		Saccharine		Bupropion		Citalopram		Carbamazepine		Gemfibrozil		Fluoxetine		Norfluoxetine		Norsertaline		Sertraline		Venlafaxine
20100706 Blnk Spk Dup	54.64	B	52.46	B	75.71	B	63.48		72		41.7		34.81		476.47	B	120.3	B	31.17		49.12		48.64		54.54		50.89		54.42		51.08		48.79		52.1
10F0882-04 Spk	56.38	B	49.8	B	264.35		87.28		131.02		52.64		25		55.03	B	61.8	B	31.49		48.38		49.03		57		49.68		47.59		<1		45.25		51.67
10F0903-06 Dup	<1		<1		252.84		2.25	B	4.58	B	0.55	BJ	<1		<1		<1		<1		<1		0.29	BJ	<1		<1		<1		<1		<1		<1
20100713 Blnk	6.79		4.64		10.8		1.54		<1		<1		<1		416.64		36.33		<1		<1		0.91		<1		<1		<1		<1		<1		<1
20100713 Blnk Spk	52.46	B	52		78.14	B	67.21		71.38		50.21		31.84		484.76	B	94.1	B	30.49		49.43		49.66		47.23		49.45		51.69		47.32		50.43		53.24
20100713 Blnk Spk Dup	54.45	B	51.31		65.04	B	76.61		78.14		41.56		34.19		453.84	B	79.66	B	31.44		49.09		49.5		46.91		50.09		45.86		54.96		47.77		52.27
10G0154-03 Spk	48.8	B	47		146.09		84.95		119.09		46.67		26.6		66.77	B	62.36	B	31.26		50.18		48.18		52.03		47.56		55.68		59.75		50.1		53.17
10G0463-01 Dup	<1		3.82	B	67.07	B	<1		1.8		0.12	BJ	<1		4.7	B	<1		<1		<1		0.2	BJ	<1		<1		<1		<1		<1		<1
20100713 Blnk	6.79		4.64		10.8		1.54		<1		<1		<1		416.64		36.33		<1		<1		0.91		<1		<1		<1		<1		<1		<1
20100719 Blnk Spk	54.97	B	52.09		82.23	B	66.96		80.64		45.02		51.33		489.95	B	80.51	B	33.33		50.09		49.51		47.71		50.32		53.31		51.72		50.48		52.67
20100719 Blnk Spk Dup	54.54	B	52.47		68.24	B	75.92		83.73		40.67		46.56		485.12	B	78	B	32.05		47.82		49.69		51.01		55.96		40.46		60.18		48.8		53.67
10G0510-02 Spk	51.23	B	45.73		217.01		95.5		154.71		45.97		46.93		63.71	B	65.12	B	34.01		49.65		49.22		51.01		50.12		56.36		55.33		50.13		54.38
10G0465-03 Dup	<1		3.39	B	86.35	B	0.54	BJ	2.29		0.11	BJ	<1		78.49	B	<1		<1		<1		0.44	BJ	<1		<1		<1		<1		<1		<1