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ELECTRONIC SUPPORTING INFORMATION FOR:

TITLE: Prioritization of suspect hits in a sensitive suspect screening workflow for comprehensive micropollutant characterization in environmental samples

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Methods – Sample Enrichment

The samples were passed over a self-packed mixed bed cartridge containing three layers separated by polyethylene frits. The bottom layer consisted of 200 mg Envi-CARB (Supelclean) media. The middle layer was 350 mg of a 1:1:1.5 (by mass) mixture of Strata X-AW (Phenomenex), Strata X-CW (Phenomenex), and Isolute ENV+ (Biotage), respectively. The final layer was 200 mg of Oasis HLB (Waters) media. This mixed bed cartridge was designed to enrich neutral, cationic, and anionic species with a broad range of polarities. The analytes were eluted using 6 mL of 50:50 v/v ethyl acetate/methanol with 0.5% ammonia, 3 mL of 50:50 v/v ethyl acetate/methanol with 1.7% formic acid, and 2 mL of pure methanol. The extracts were evaporated under a stream of high-purity nitrogen to 100 µL and reconstituted to 1 mL using nanopure water. The extracted samples were filtered (regenerated cellulose, 0.45 µm, Thermo Scientific) and stored at -20 ˚C and in the dark until analysis.

Methods - Analytical method

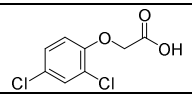
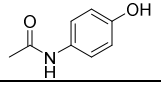
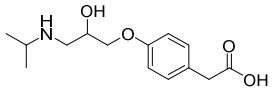
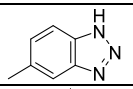
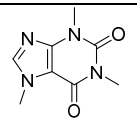
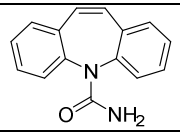
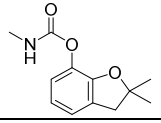
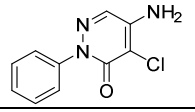
Samples were injected into the column at 20 µL with an initial mobile phase of 90% A and elution from the column was achieved with a final mobile phase of 5% A. An eluent gradient was used to achieve separation of analytes. The percentage of A was linearly decreased to 50% over four minutes, and then linearly decreased to 5% A for thirteen minutes; the gradient was then held at 5% A for eight minutes before returning to 90% A and remaining at that point until the end of the separation method at 29 minutes. Mass calibrations and mass accuracy checks were performed before each sequence of measurements; resolution was always greater than 140,000 (at mass of 200) and mass accuracy was always within ±1 ppm.

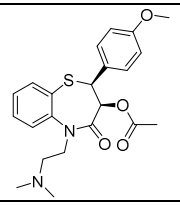
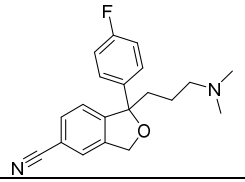
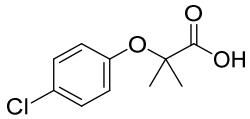
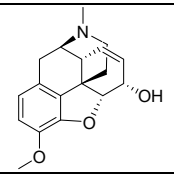
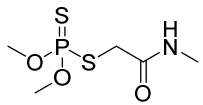
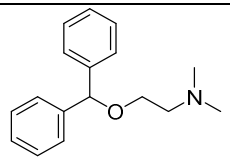
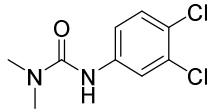
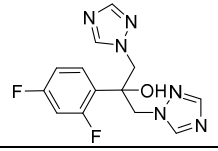
Table ES-1. QExactive method parameters for full scan MS acquisition and data-dependent MS2 experiments.

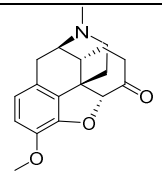
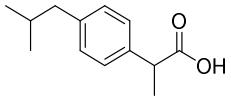
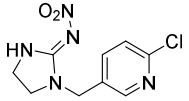
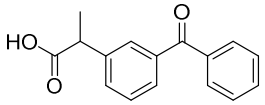
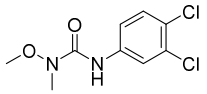
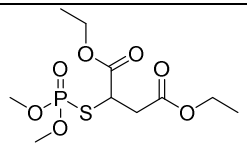
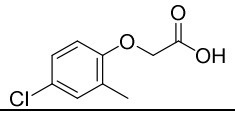
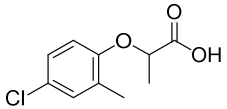
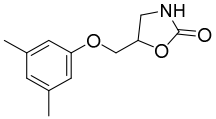
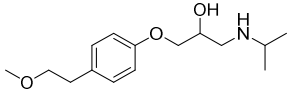
Parameter		Value
Voltage (pos/neg)		4kV/3kV
Sheath gas		40
Aux gas		20
Capillary temperature		320°C
Source temperature		50°C
Full MS	Resolution	140,000
	Polarity	Positive/Negative Switching
	AGC Target	5e5
	Maximum IT	250 ms
	Scan range	100 to 1000 m/z
dd-MS^2	Resolution	17,500
	AGC target	2e5
	Maximum IT	100 ms
	Loop count	5
	Isolation window	1.0 m/z
	Dynamic exclusion	8 sec

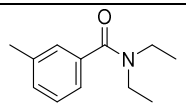
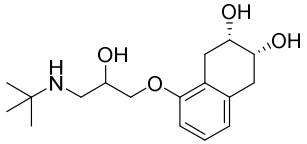
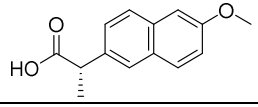
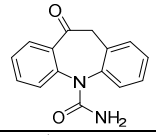
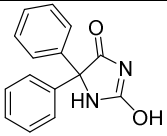
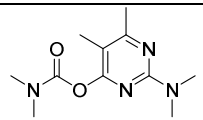
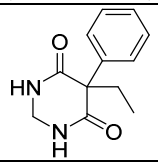
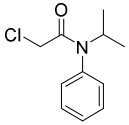
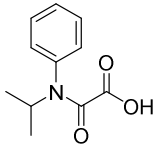
Methods - Validation compounds

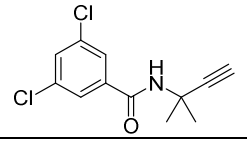
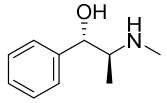
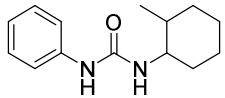
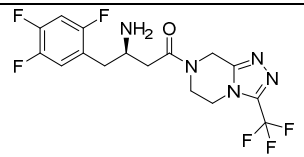
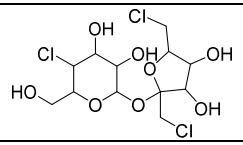
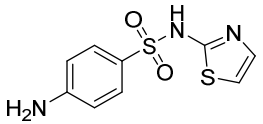
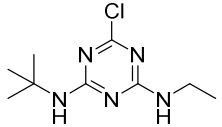
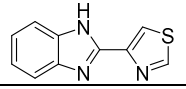
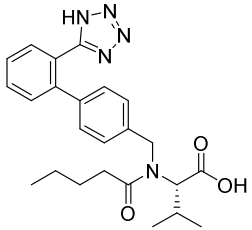
Table ES-2. Names, structures, compound class, and analytical details for the 45 validation compounds.

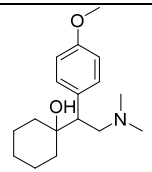
Compound	CAS No.	Compound Class	Structure	Accurate Mass & Adduct	RT (min)	Fragments
2,4-D	94-75-7	Pesticide		218.9621 [M-H]-	8.1	160.96, 124.98
Acetaminophen	103-90-2	Pharm		152.0706 [M+H]+	2.3	110.06, 93.04, 65.04
Atenolol Acid	56392-14-4	Pharm		268.1543 [M+H]+	3.3	145.06, 191.07, 226.11
5-methyl-1H-benzotriazole	136-85-6	Other		134.0713 [M+H]+	5.1	106.07, 53.04, 79.05
Caffeine	58-08-2	Lifestyle		195.0877 [M+H]+	3.4	138.07, 110.07, 84.96
Carbamazepine	298-46-4	Pharm		237.1022 [M+H]+	6.6	194.10, 192.08
Carbofuran	1563-66-2	Pesticide		222.1125 [M+H]+	6.05	123.04, 165.09, 137.06
Chloridazon	1698-60-8	Pesticide		222.0429 [M+H]+	4.5	104.05, 92.05, 146.01

cis-Diltiazem	42399-41-7	Pharm		415.1693 [M+H]+	6.4	310.09, 178.03
Citalopram	59729-33-8	Pharm		325.1711 [M+H]+	5.9	109.04, 262.10, 234.07
Clofibric Acid	882-09-7	Pharm		213.0324 [M-H]-	8.9	126.99, 85.08
Codeine	76-57-3	Pharm		300.1594 [M+H]+	2.52	215.11, 243.10
Dimethoate	60-51-5	Pesticide		230.0069 [M+H]+	4.5	142.99, 170.97, 88.02
Diphenhydramine	58-73-1	Pharm		256.1701 [M+H]+	5.95	167.09, 152.06
Diuron	330-54-1	Pesticide		233.0243 [M+H]+	7.9	137.07, 94.07, 177.06
Fluconazole	86386-73-4	Pharm		307.1113 [M+H]+	4.5	220.07, 238.08, 169.05

Hydrocodone	125-29-1	Pharm		300.1599 [M+H]+	2.84	199.08, 241.09
Ibuprofen	15687-27-1	Pharm		229.0864 [M+Na]+	11.9	151.04, 101.06, 83.05
Imidacloprid	138261-41-3	Pesticide		256.0596 [M+H]+	4.0	175.10, 209.06, 128.03
Ketoprofen	22071-15-4	Pharm		255.1016 [M+H]+	8.45	105.04, 209.10, 177.05
Linuron	330-55-2	Pesticide		249.0192 [M+H]+	8.9	159.97, 182.02, 160.98
Malaoxon	1634-78-2	Pesticide		315.0667 [M+H}+	6.2	99.01, 127.04, 142.99
MCPA	94-74-6	Pesticide		199.0156 [M-H]-	8.4	141.01
Mecoprop	93-65-2	Pesticide		213.0324 [M-H]-	9.7	141.01
Metaxalone	1665-48-1	Pharm		222.1125 [M+H]+	7.05	133.10, 105.07, 161.10
Metoprolol	37350-58-6	Pharm		268.1907 [M+H}+	4.5	191.11, 159.08, 116.11

DEET	134-62-3	Pesticide		192.1383 [M+H]+	7.5	119.05, 91.05, 72.04
Nadolol	42200-33-9	Pharm		310.2013 [M+H]+	3.55	254.14, 201.09, 236.13
Naproxen	22204-53-1	Pharm		231.1016 [M+H]+	9.0	175.06, 185.10, 170.07
Oxcarbazepine	28721-07-5	Pharm		253.0972 [M+H]+	5.7	208.08, 180.08, 236.07
Phenytoin	57-41-0	Pharm		253.0977 [M+H]+	6.5	182.10, 104.05
Pirimicarb	23103-98-2	Pesticide		239.1503 [M+H]+	4.1	72.04, 137.07, 182.13
Primidone	125-33-7	Pharm		219.1128 [M+H]+	4.6	91.05, 162.09, 119.09
Propachlor	1918-16-7	Pesticide		212.0837 [M+H]+	7.5	170.04, 94.07, 106.07
Propachlor-OXA	70628-36-3	Pesticide		208.0968 [M+H]+	4.8	120.04, 92.05

Propyzamide	23950-58-5	Pesticide		256.0296 [M+H]+	9.6	189.98, 172.96, 67.05
Pseudoephedrine	299-42-3	Pharm		166.1229 [M+H]+	2.8	133.09, 148.11, 117.07
Siduron	1982-49-6	Pesticide		233.1654 [M+H]+	8.9	137.07, 94.07, 120.04
Sitagliptin	486460-32-6	Pharm		408.1254 [M+H]+	4.6	235.08, 174.05, 193.07
Sucralose[a]	56038-13-2	Lifestyle		441.0128 [M+FA]-	3.9	185.02, 121.03
Sulfathiazole	72-14-0	Pharm		256.0209 [M+H]+	2.6	156.01, 108.04, 68.05
Terbutylazine	5915-41-3	Pesticide		230.1167 [M+H]+	9.0	174.05
Thiabendazole	148-79-8	Pharm		202.0433 [M+H]+	3.45	175.03, 131.06
Valsartan	137862-53-4	Pharm		436.2343 [M+H]+	9.7	235.10, 291.19, 207.09

Venlafaxine	93413-69-5	Pharm		278.2115 [M+H]+	5.5	121.06, 147.08, 58.07

[a]The $[M+FA]^-$ adduct was identified as the most intense adduct for sucralose during compound tuning and was therefore used for sample screening.

Results – Development and optimization of suspect screening workflow

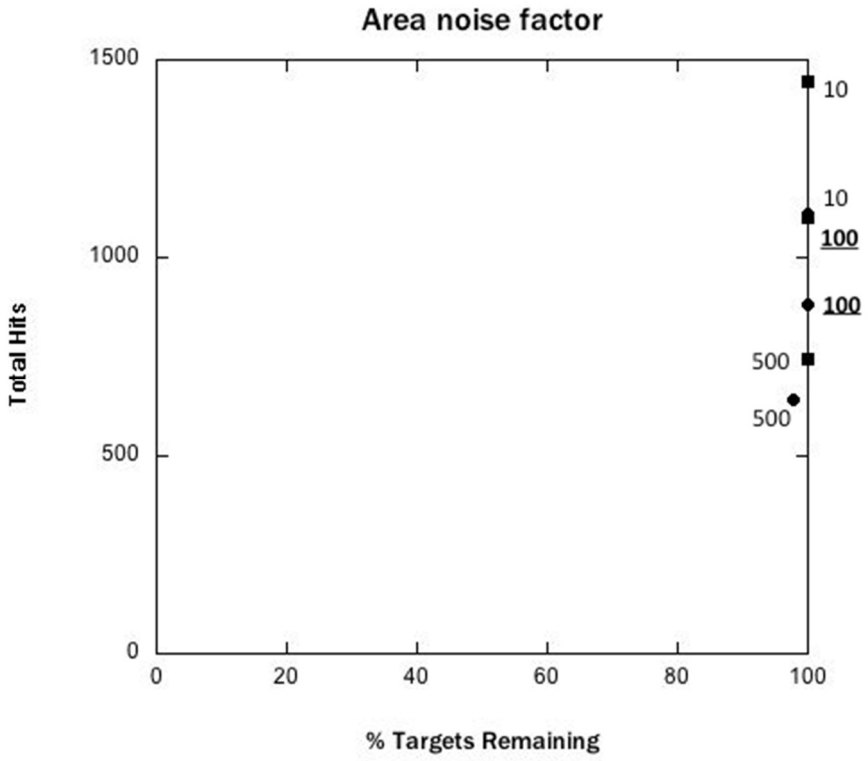


Figure ES-1. Optimization graph for area noise factor; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Optimized value of 100 is shown underlined and bolded.

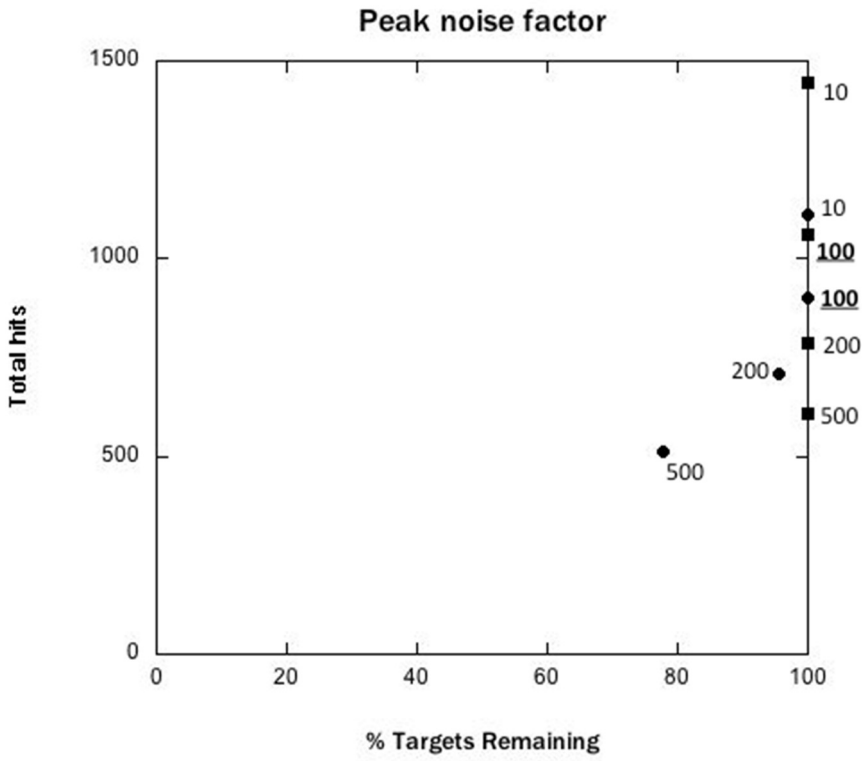


Figure ES-2. Optimization graph for peak noise factor; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Optimized value of 100 is shown underlined and bolded.

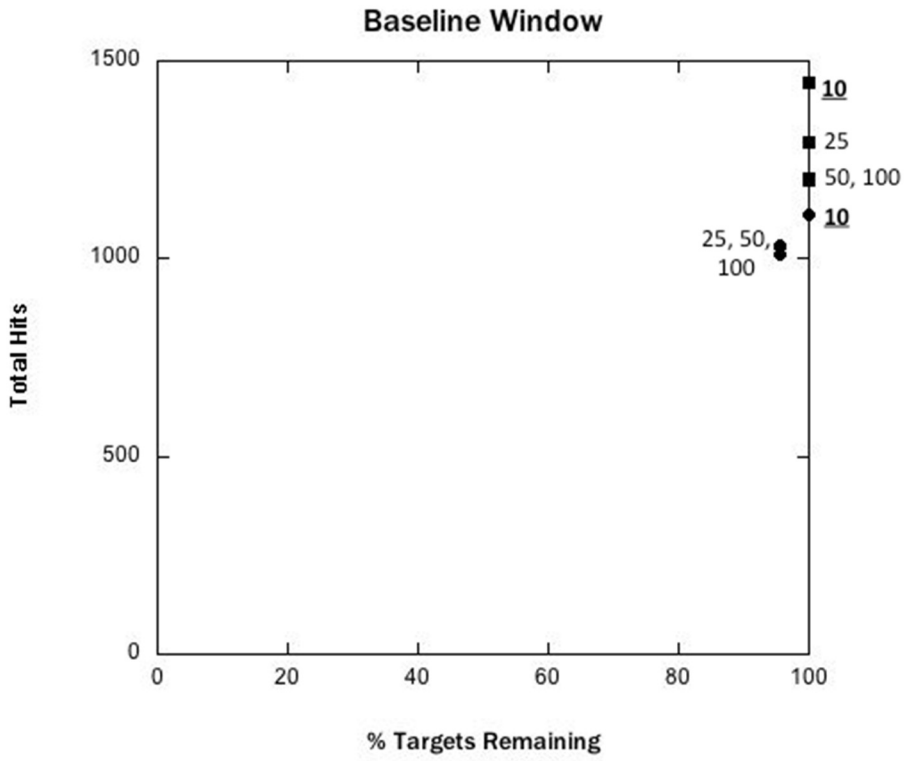


Figure ES-3. Optimization graph for baseline window; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Optimized value of 10 is shown underlined and bolded.

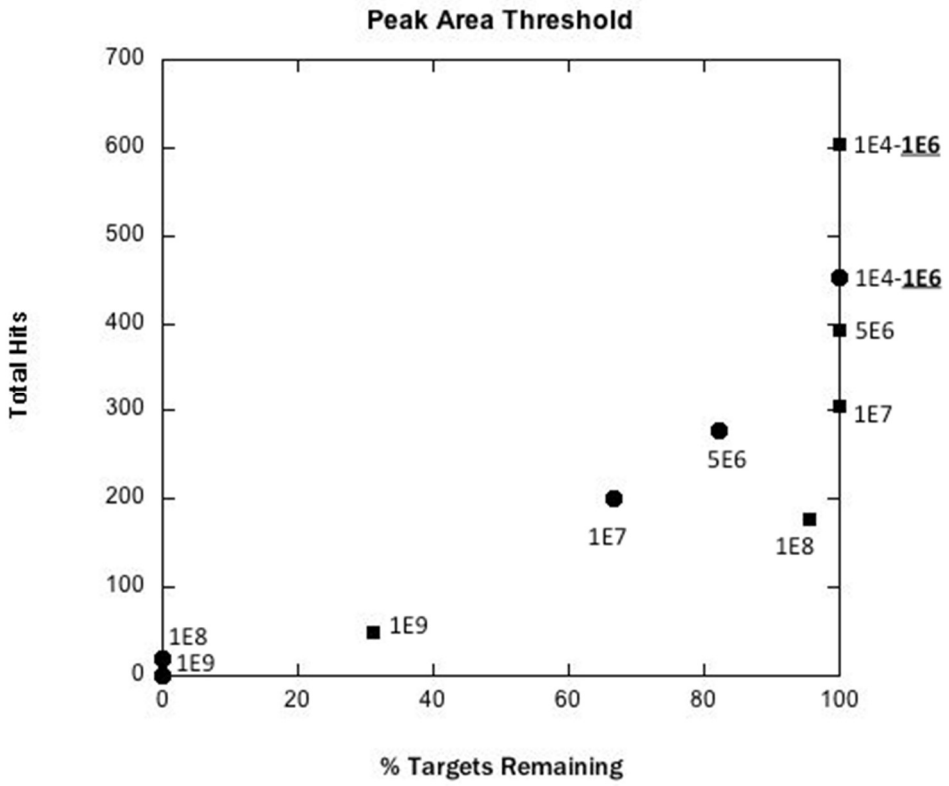


Figure ES-4. Optimization graph for peak area threshold; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Optimized value of 1E6 is shown underlined and bolded.

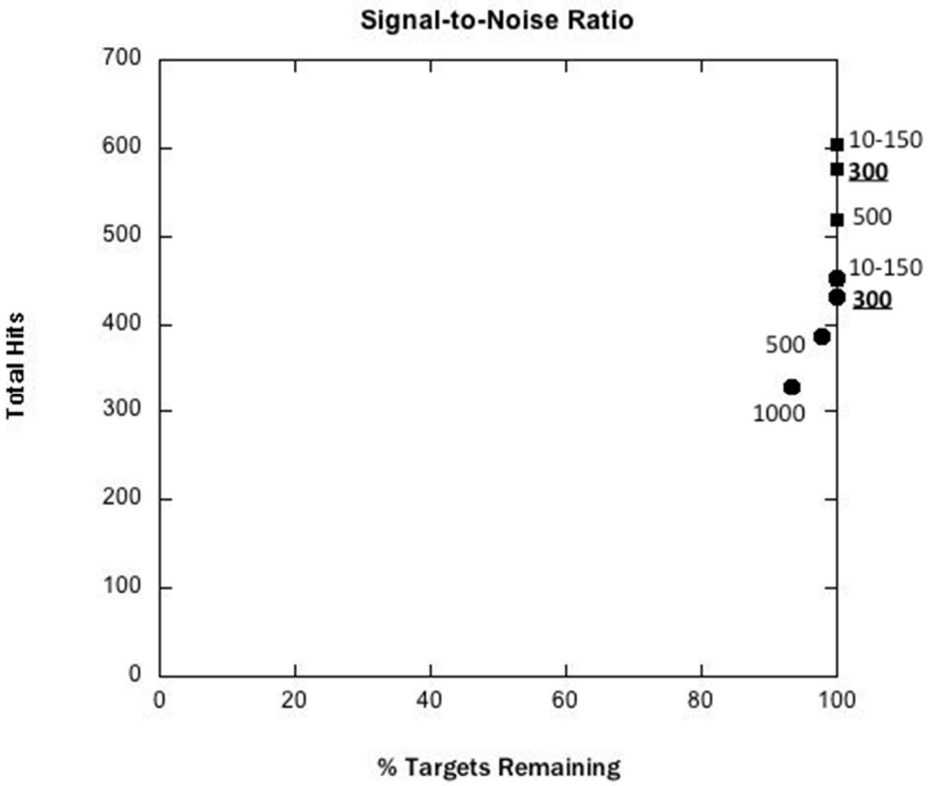


Figure ES-5. Optimization graph for signal-to-noise threshold; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Optimized value of 300 is shown underlined and bolded.

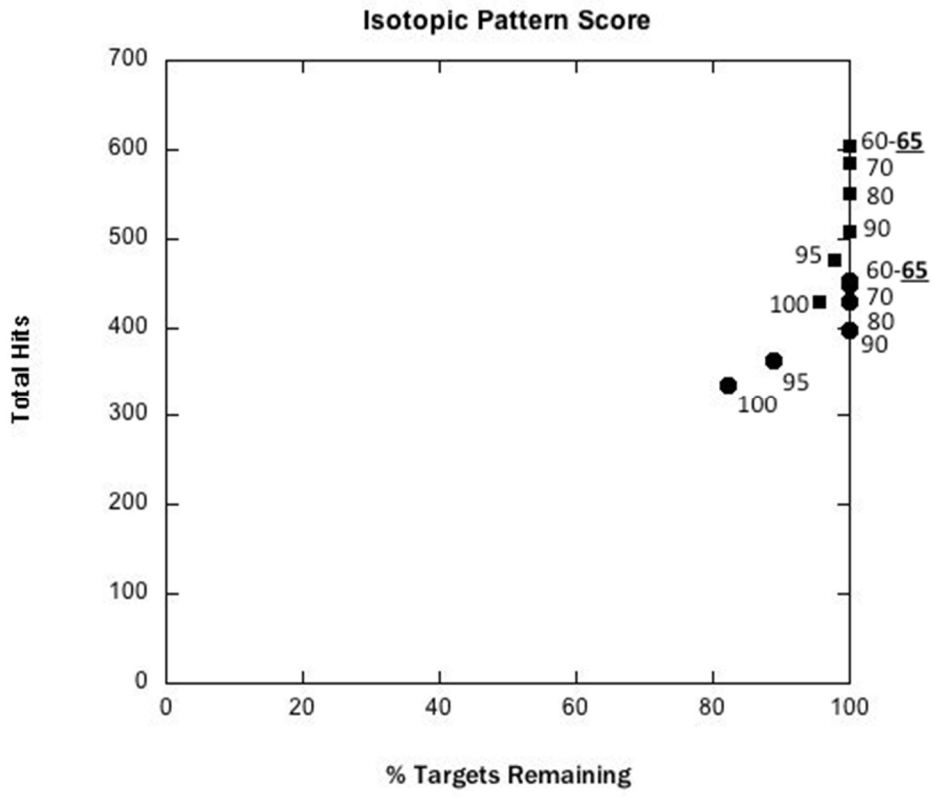


Figure ES-6. Optimization graph for isotopic pattern score; low (25 ng/L) and high (750 ng/L) concentration samples are represented as circles and squares, respectively. Chosen value of 65% is shown bolded and underlined.

Table ES-3. ICIS peak detection parameters isotopic pattern parameters used in TraceFinder v3.1.

Peak Detection Parameters	Value
Detection method	All
Smoothing	1
Area noise factor	100
Peak noise factor	100
Baseline window	10
Noise method	Incos
Min peak width	5
Multiplet resolution	10
Area tail extension	5
Area scan window	0
Peak area threshold	1E6
Signal-to-noise ratio	300
Isotopic Pattern Parameters	
Isotopic pattern fit threshold (%)	65
Allowed mass deviation (ppm)	10
Allowed intensity deviation (%)	10

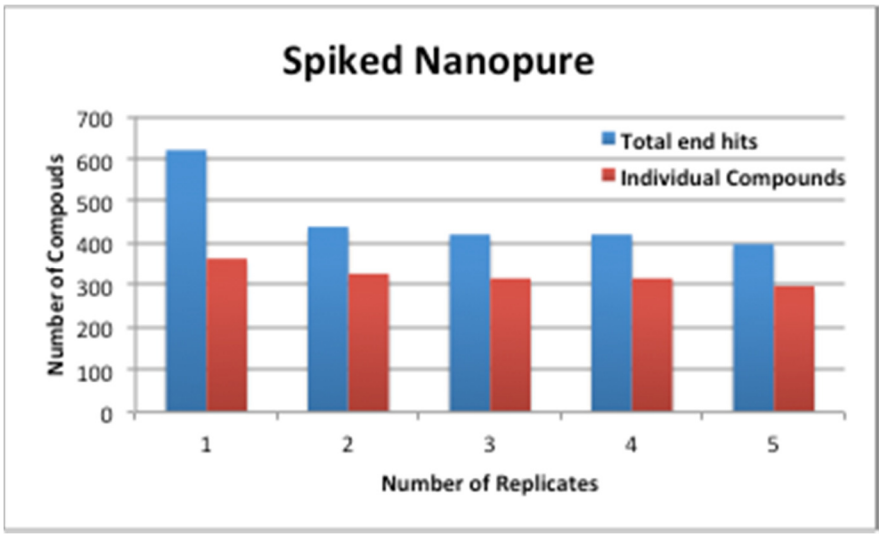


Figure ES-7. Optimization graph for the replication filter; the total number of suspect hits (blue bars) and the number of unique suspect hits (red bars) approached a steady-state at three replicate injections.

Results – Application of suspect screening workflow

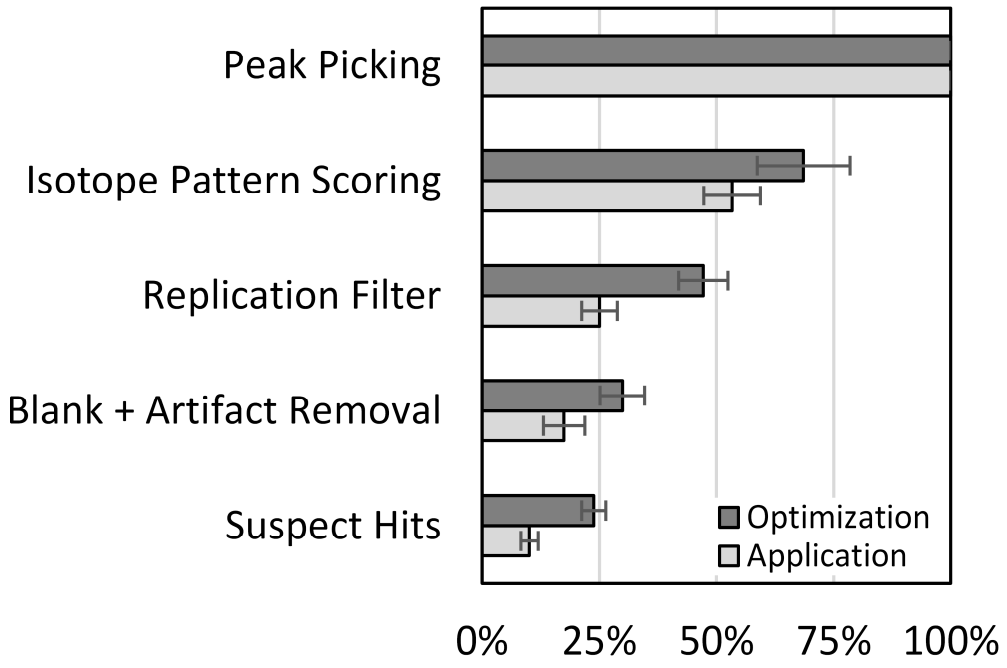


Figure ES-8. Comparison of the percent reduction in suspect hits for the application samples and optimization samples after each step in the suspect screening workflow.

Results – Prioritization strategies

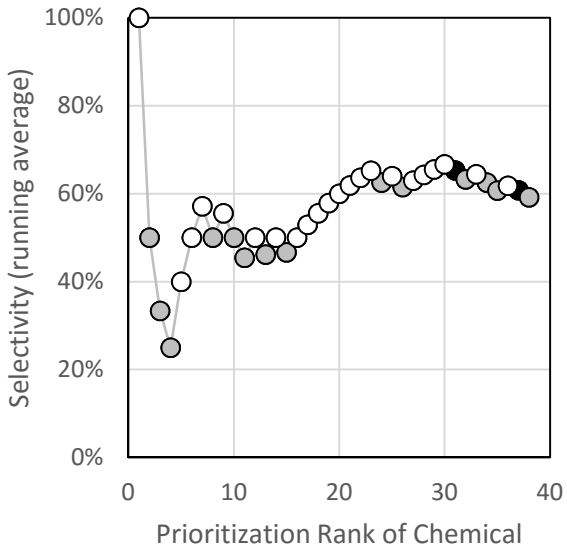


Figure ES-9. The running selectivity versus the prioritization rank of the chemical for the WOS prioritization strategy. A total of 38 suspect hits were on the prioritization list with 22 confirmations (white circles), 14 failed confirmations (gray circles), and 2 suspect hits for which authentic standards were not acquired (black circles).

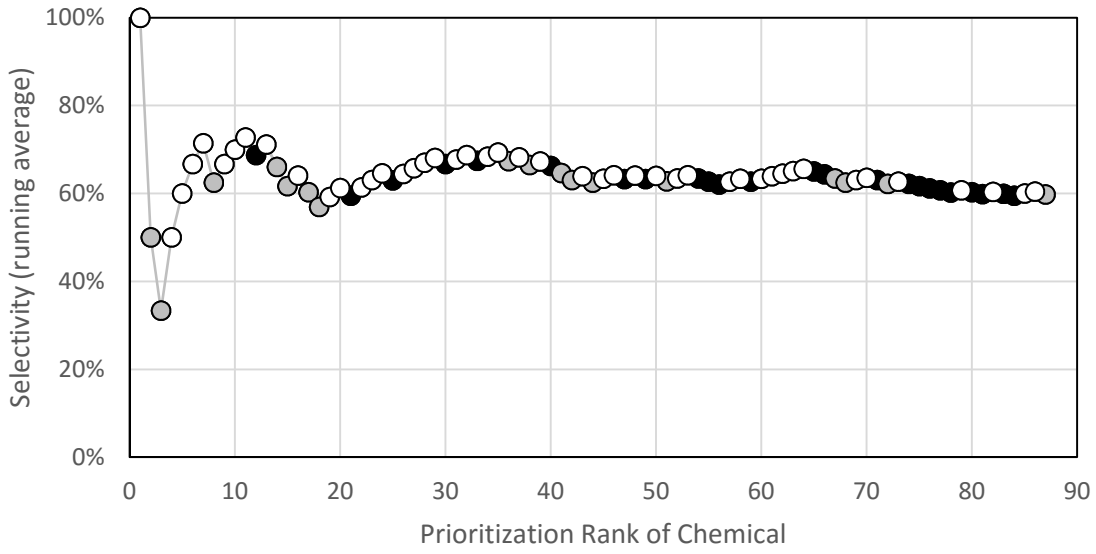


Figure ES-10. The running selectivity versus the prioritization rank of the chemical for the WOS + WWTPs prioritization strategy. A total of 87 suspect hits were on the prioritization list with 46 confirmations (white circles), 17 failed confirmations (gray circles), and 24 suspect hits for which authentic standards were not acquired (black circles).

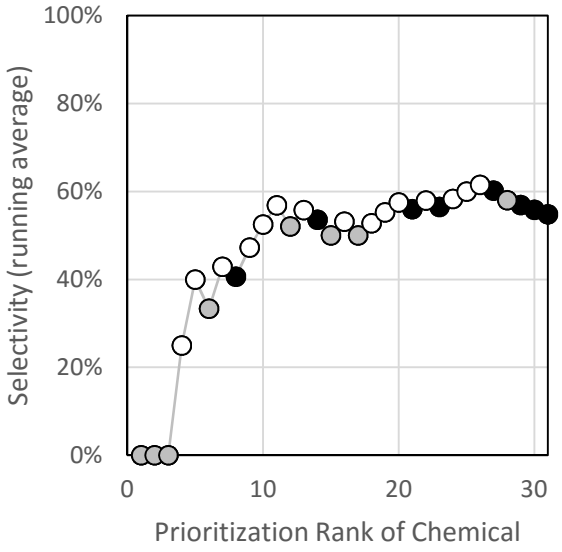


Figure ES-11. The running selectivity versus the prioritization rank of the chemical for the WOS + lake prioritization strategy. A total of 30 suspect hits were on the prioritization list with 15 confirmations (white circles), 8 failed confirmations (gray circles), and 7 suspect hits for which authentic standards were not acquired (black circles).

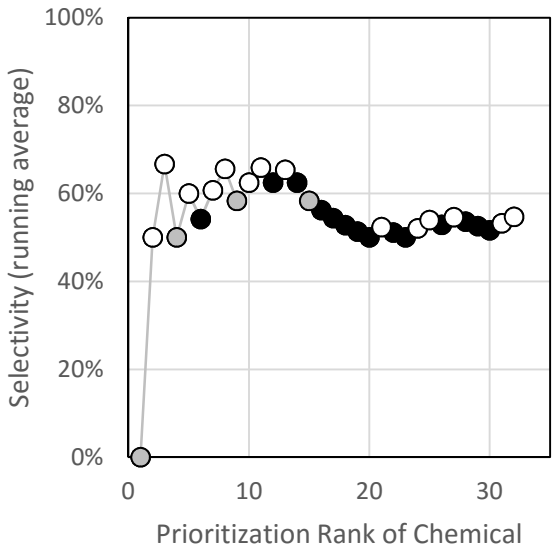


Figure ES-12. The running selectivity versus the prioritization rank of the chemical for the WOS + DWTP intake prioritization strategy. A total of 32 suspect hits were on the prioritization list with 14 confirmations (white circles), 4 failed confirmations (gray circles), and 14 suspect hits for which authentic standards were not acquired (black circles).

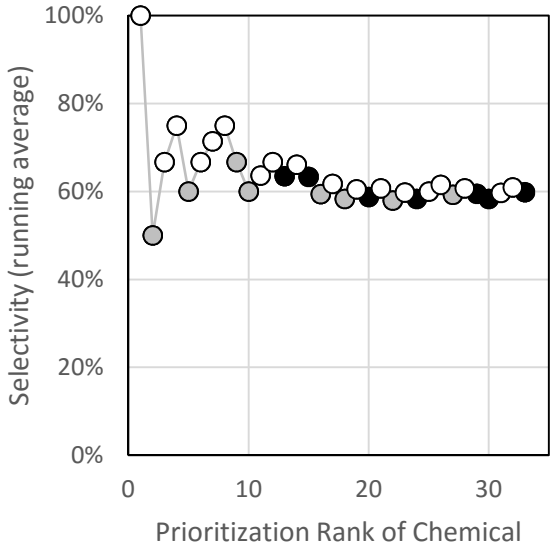


Figure ES-13. The running selectivity versus the prioritization rank of the chemical for the WOS + chlorine atom prioritization strategy. A total of 33 suspect hits were on the prioritization list with 18 confirmations (white circles), 8 failed confirmations (gray circles), and 7 suspect hits for which authentic standards were not acquired (black circles).

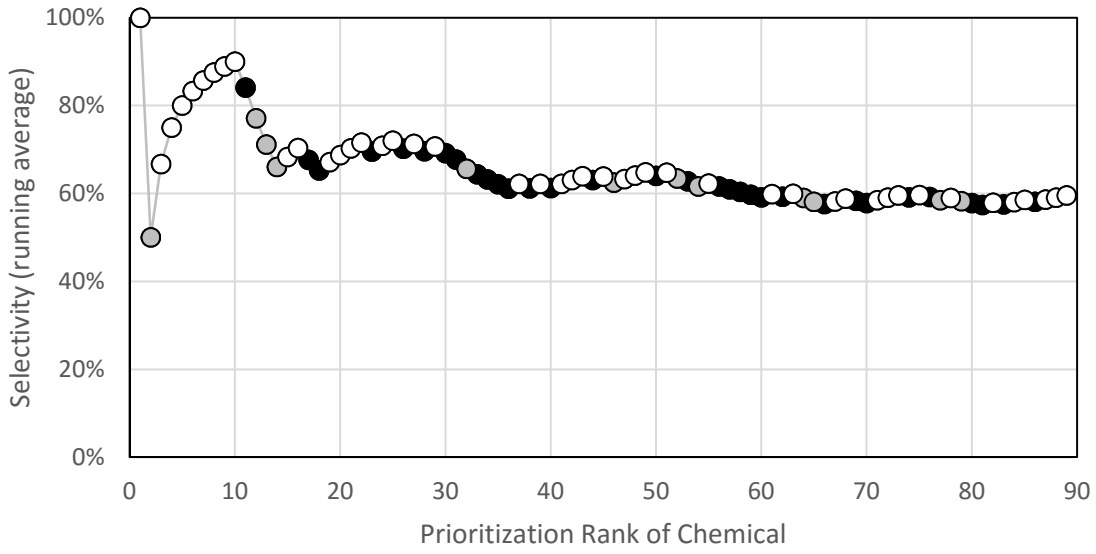


Figure ES-14. The running selectivity versus the prioritization rank of the chemical for the WOS + USGS prioritization strategy. A total of 89 suspect hits were on the prioritization list with 45 confirmations (white circles), 12 failed confirmations (gray circles), and 32 suspect hits for which authentic standards were not acquired (black circles).

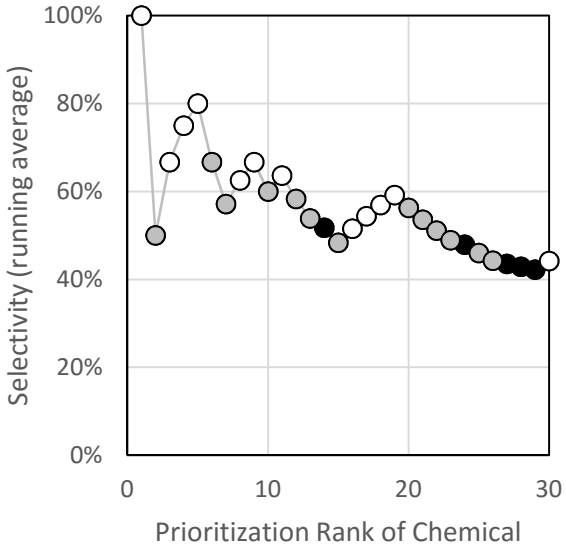


Figure ES-15. The running selectivity versus the prioritization rank of the chemical for the WOS + PPIMS strategy. A total of 30 suspect hits were on the prioritization list with 12 confirmations (white circles), 13 failed confirmations (gray circles), and 5 suspect hits for which authentic standards were not acquired (black circles).

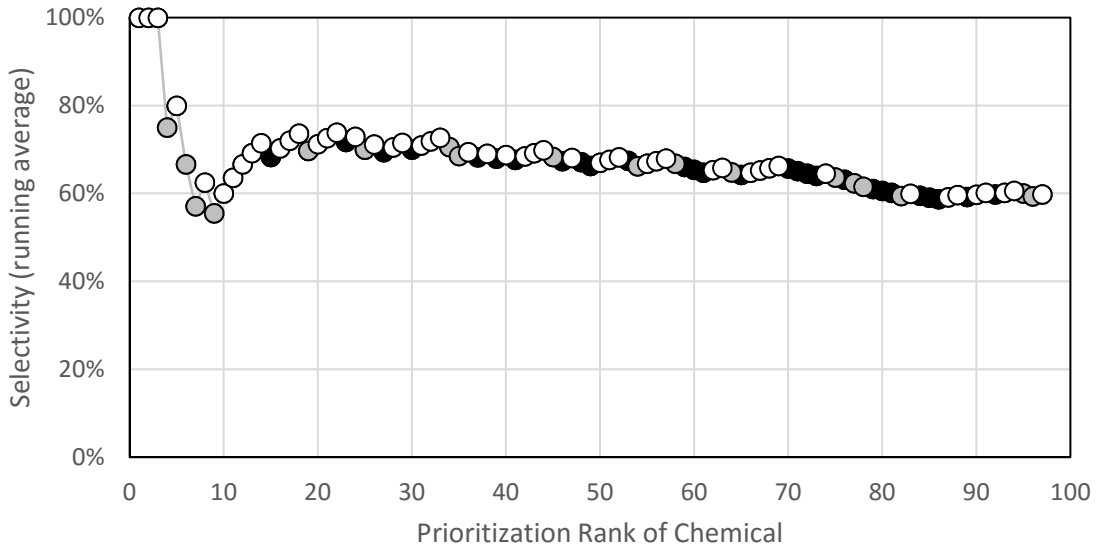


Figure ES-16. The running selectivity versus the prioritization rank of the chemical for the WOS + WWTPs + pharmaceuticals strategy. A total of 97 suspect hits were on the prioritization list with 51 confirmations (white circles), 18 failed confirmations (gray circles), and 28 suspect hits for which authentic standards were not acquired (black circles).

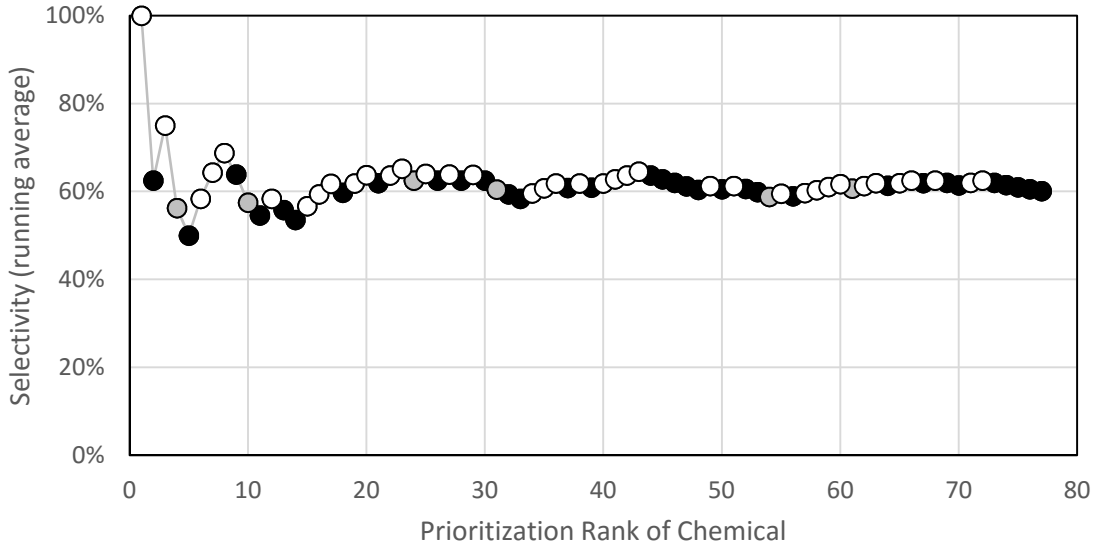


Figure ES-17. The running selectivity versus the prioritization rank of the chemical for the peak area prioritization strategy. A total of 77 suspect hits were on the prioritization list with 38 confirmations (white circles), 6 failed confirmations (gray circles), and 33 suspect hits for which authentic standards were not acquired (black circles).

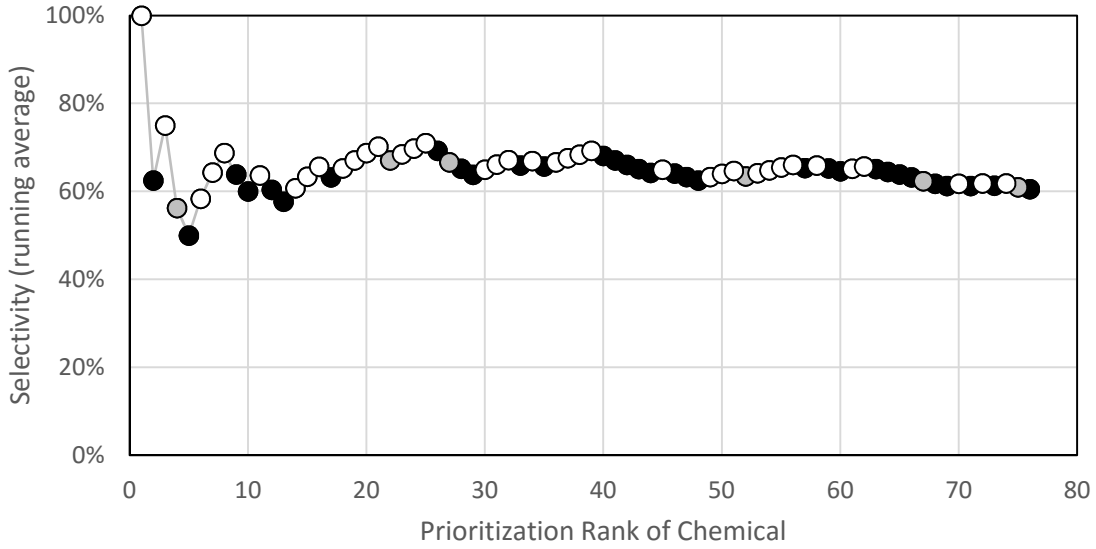


Figure ES-18. The running selectivity versus the prioritization rank of the chemical for the peak area + WWTPs prioritization strategy. A total of 78 suspect hits were on the prioritization list with 38 confirmations (white circles), 6 failed confirmations (gray circles), and 34 suspect hits for which authentic standards were not acquired (black circles).

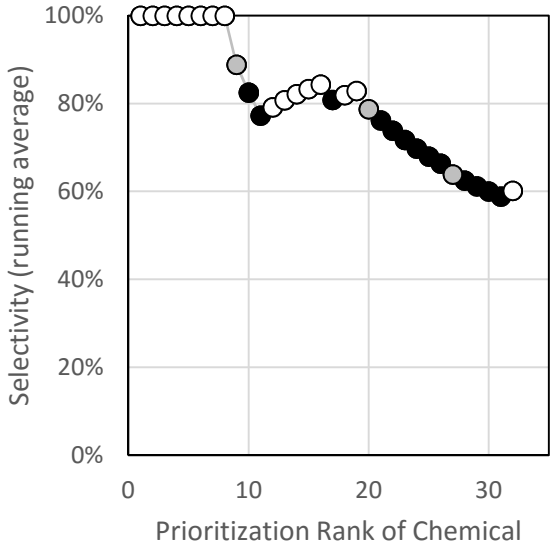


Figure ES-19. The running selectivity versus the prioritization rank of the chemical for the peak area + lake prioritization strategy. A total of 32 suspect hits were on the prioritization list with 16 confirmations (white circles), 3 failed confirmations (gray circles), and 13 suspect hits for which authentic standards were not acquired (black circles).

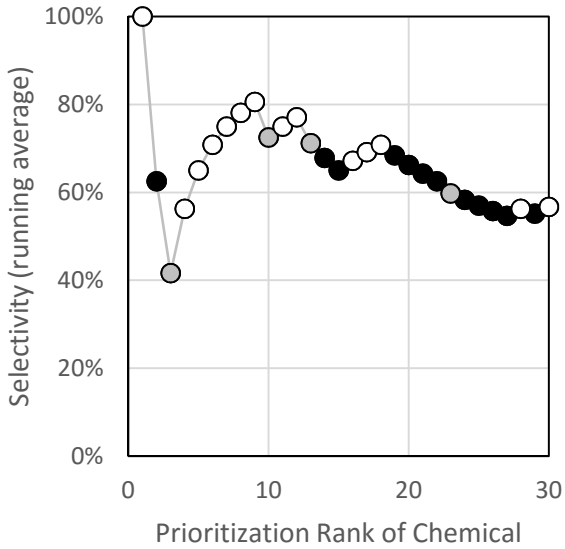


Figure ES-20. The running selectivity versus the prioritization rank of the chemical for the peak area + DWTP intake prioritization strategy. A total of 30 suspect hits were on the prioritization list with 14 confirmations (white circles), 6 failed confirmations (gray circles), and 12 suspect hits for which authentic standards were not acquired (black circles).

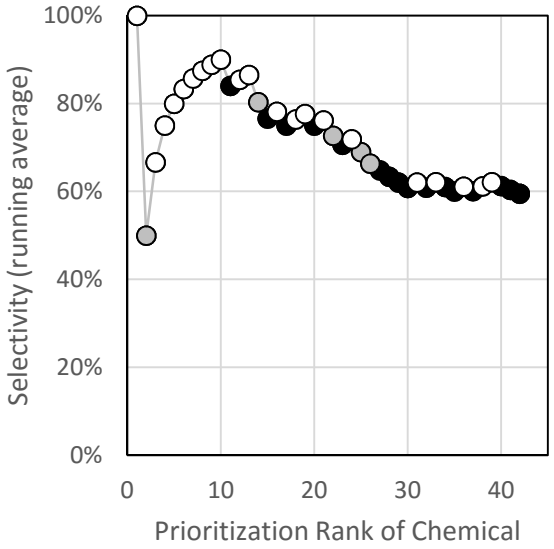


Figure ES-21. The running selectivity versus the prioritization rank of the chemical for the peak area + chlorine atom prioritization strategy. A total of 42 suspect hits were on the prioritization list with 21 confirmations (white circles), 5 failed confirmations (gray circles), and 16 suspect hits for which authentic standards were not acquired (black circles).

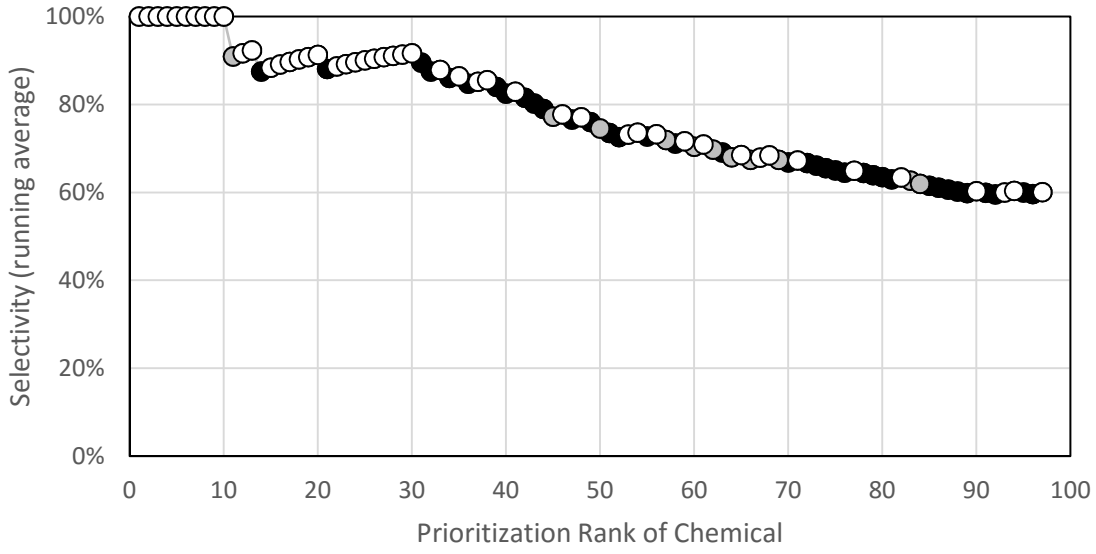


Figure ES-22. The running selectivity versus the prioritization rank of the chemical for the peak area + USGS prioritization strategy. A total of 97 suspect hits were on the prioritization list with 49 confirmations (white circles), 11 failed confirmations (gray circles), and 37 suspect hits for which authentic standards were not acquired (black circles).

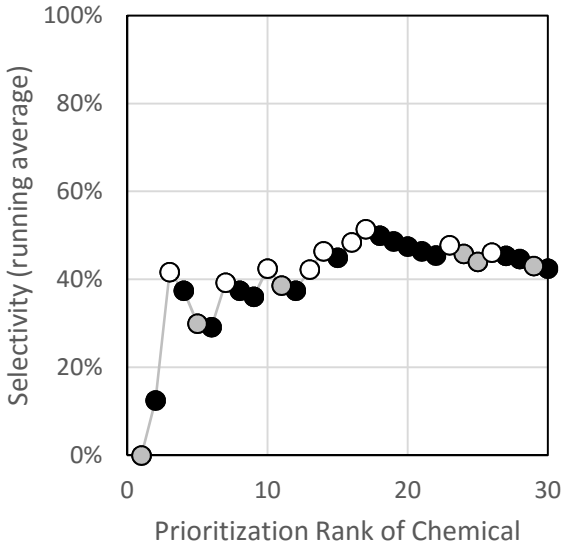


Figure ES-23. The running selectivity versus the prioritization rank of the chemical for the peak area + PPIMS strategy. A total of 30 suspect hits were on the prioritization list with 9 confirmations (white circles), 6 failed confirmations (gray circles), and 15 suspect hits for which authentic standards were not acquired (black circles).

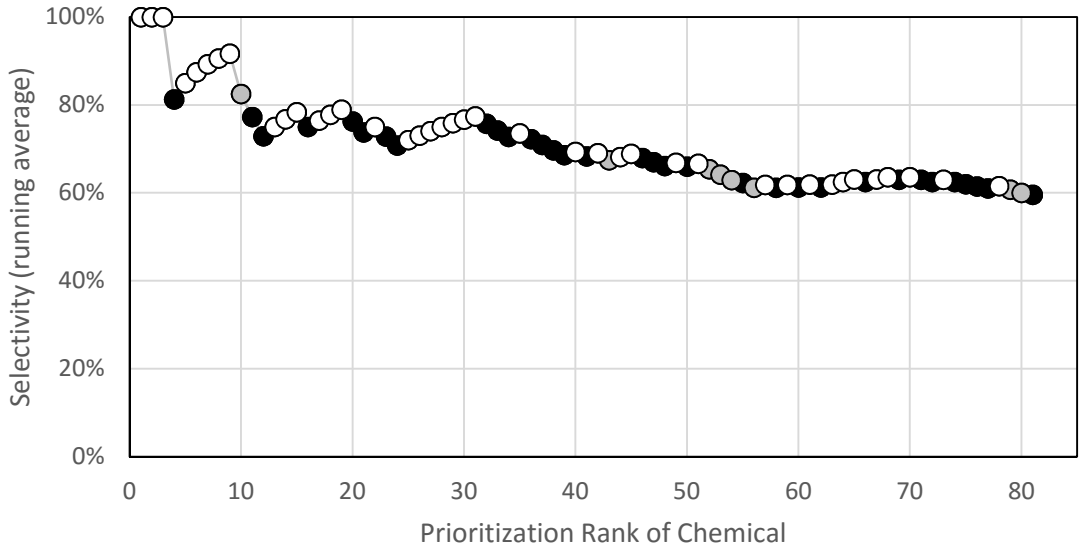


Figure ES-24. The running selectivity versus the prioritization rank of the chemical for the peak area + WWTPs + pharmaceuticals strategy. A total of 81 suspect hits were on the prioritization list with 40 confirmations (white circles), 8 failed confirmations (gray circles), and 33 suspect hits for which authentic standards were not acquired (black circles).

Results – Investigated compounds

Table ES-4. List of 172 suspect hits that were compared with an authentic standard along with analytical details and confirmed/failed status.

Compound	Chemical Formula	Status	Accurate Mass[a]	RT (min)	Fragments
10,11-dihydrocarbamazepine	C15H14N2O	Failed	239.1170 [M+H]+	7.0	194.10
1H-Benzotriazole	C6H5N3	Confirmed	120.0556 [M+H]+	3.9	92.05, 65.04
2-Aminobenzimidazole	C7H7N3	Failed	134.0713 [M+H]+	2.67	92.05, 107.06
2,4-D	C8H6Cl2O3	Confirmed	218.9621 [M-H]-	8.1	160.96, 124.98
5-Methyl-1H-benzotriazole	C7H7N3	Confirmed	134.0713 [M+H]+	5.1	106.07, 53.04, 79.05
Abacavir	C14H18N6O	Confirmed	287.1620 [M+H]+	3.35	191.10, 150.06, 79.05
Abscisic Acid	C15H20O4	Failed	265.1434 [M+H]+	6.13	135.080, 187.11, 173.13
Acesulfame	C4H5NO4S	Confirmed	161.9856 [M-H]-	1.7	82.03, 77.96
Acetaminophen	C8H9NO2	Confirmed	152.0706 [M+H]+	2.3	110.06, 93.03, 65.04
Adenosine	C10H13N5O4	Confirmed	268.1037 [M+H]+	1.5	136.06
Albuterol	C13H21NO3	Confirmed	240.1594 [M+H]+	2.18	148.07, 121.06
Allopurinol	C5H4N4O	Confirmed	137.0463 [M+H]+	1.47	110.04, 120.02, 72.94
Amisulpride	C17H27N3O4S	Failed	370.1795 [M+H]+	3.21	242.05, 112.11
Amitriptyline	C20H23N	Failed	278.1903 [M+H]+	7.75	233.13, 191.09, 91.05

Amphetamine	C9H13N	Confirmed	136.1121 [M+H]+	3.3	91.05
Aspirin	C9H8O4	Failed	179.0344 [M-H]-	4.9	93.03, 122.96, 59.01
Atenolol	C14H22N2O3	Confirmed	267.1703 [M+H]+	2.3	190.089, 145.06, 116.11
Atenolol acid	C14H21NO4	Confirmed	268.1543 [M+H]+	3.3	145.06, 191.07, 226.11
Atomoxetine	C17H21NO	Failed	256.1696 [M+H]+	7.05	224.08, 148.11, 117.07
Atrazine	C8H14Cl1N5	Confirmed	216.1011 [M+H]+	7.3	174.05, 132.03, 104.00
Atrazine-2-hydroxy	C8H15N5O	Confirmed	198.1349 [M+H]+	3.8	156.09, 114.07, 86.04
Atrazine-desethyl	C6H10ClN5	Confirmed	188.0697 [M+H]+	4.8	146.02, 104.00, 79.01
Atropine	C17H23NO3	Failed	290.1751 [M+H]+	3.72	124.11, 93.07
Azoxystrobin	C22H17N3O5	Failed	404.1241 [M+H]+	8.7	372.10, 344.10, 316.11
Bentazone	C10H12N2O3S	Confirmed	239.0496 [M-H]-	6.6	132.03, 175.09, 197.00
Benzophenone	C13H10O	Confirmed	183.0809 [M+H]+	9	105.03, 53.04
Benzophenone-3	C14H12O3	Confirmed	229.0864 [M+H]+	10.95	151.04, 105.03
Benzothiazole	C7H5NS	Confirmed	136.0221 [M+H]+	5.65	136.02, 109.01
Benzoylecgonine	C16H19NO4	Confirmed	290.1387 [M+H]+	4	168.10, 105.03, 150.09
Benzyladenine	C12H11N5	Failed	226.1092 [M+H]+	4.6	91.05, 148.06
Bifenazate	C17H20N2O3	Failed	301.1552 [M+H]+	10.06	174.06, 222.96, 146.06

Bupropion	C13H18ClNO	Confirmed	240.1156 [M+H]+	5.1	131.07, 166.04, 184.05
Caffeine	C8H10N4O2	Confirmed	195.0877 [M+H]+	3.4	138.07, 110.07, 84.96
Camphor	C10H16O	Failed	153.1274 [M+H]+	8.15	97.07, 69.07
Carbamazepine	C15H12N2O	Confirmed	237.1022 [M+H]+	6.6	194.10, 192.08
Carbamazepine-10,11-epoxide	C15H12N2O2	Confirmed	253.0972 [M+H]+	5.32	180.08, 182.10, 210.09
Carbaryl	C12H11NO2	Failed	202.0863 [M+H]+	6.6	145.06, 155.06, 117.07
Carbendazim	C9H9N3O2	Confirmed	192.0768 [M+H]+	3.06	160.05, 132.06
Carbofuran	C12H15NO3	Failed	222.1125 [M+H]+	6.05	123.04, 165.09, 137.06
Carisoprodol	C12H24N2O4	Confirmed	261.1815 [M+H]+	7.6	97.10, 62.02, 158.12
Cetirizine	C21H25ClN2O3	Confirmed	389.1626 [M+H]+	8.3	201.05
Cimetidine	C10H16N6S	Confirmed	253.1236 [M+H]+	2.3	150.09, 159.07, 117.05
Ciprofloxacin	C17H18FN3O3	Confirmed	332.1405 [M+H]+	3.78	245.11, 288.15, 268.14
Citalopram	C20H21FN2O	Failed	325.1711 [M+H]+	5.9	109.04, 262.10, 234.07
Citric Acid	C6H8O7	Confirmed	191.0186 [M-H]-	1.26	111.01, 87.01, 123.95
Clarithromycin	C38H69NO13	Confirmed	748.4842 [M+H]+	8.75	157.12, 590.39, 558.36
Clindamycin	C18H33ClN2O5S	Confirmed	425.1877 [M+H]+	5.95	126.13, 377.18
Clofibric acid	C10H11ClO3	Failed	213.0324 [M-H]-	8.9	126.99, 85.03

Codeine	C18H21NO3	Confirmed	300.1594 [M+H]+	2.52	215.11, 243.10
Corticosterone	C21H30O4	Failed	347.2217 [M+H]+	8.2	121.07, 145.10, 97.07
Cotinine	C10H12N2O	Confirmed	177.1028 [M+H]+	1.2	80.05, 98.06, 146.06
DEET	C12H17NO	Confirmed	192.1383 [M+H]+	7.5	119.05, 91.05, 72.04
Desvenlafaxine	C16H25NO2	Confirmed	264.1958 [M+H]+	4.24	133.06, 107.05, 58.07
Dextromethorphan	C18H25NO	Confirmed	272.2009 [M+H]+	5.8	215.14, 147.08
Dicamba	C8H6Cl2O3	Failed	218.9621 [M-H]-	6.1	89.02
Diclofenac	C14H11Cl2NO2	Confirmed	296.0240 [M+H]+	11.5	215.05, 250.02, 184.02
Diethyl-phthalate	C12H14O4	Confirmed	223.0965 [M+H]+	7.72	149.02, 121.03
Dihydroxycarbamaz-epine	C15H14N2O3	Failed	239.1179 [M+H]+	7.02	194.10, 196.11, 222.09
cis-Diltiazem	C22H26N2O4S	Confirmed	415.1692 [M+H]+	6.4	310.09, 178.03
Dimethachlor	C13H18ClNO2	Failed	256.1099 [M+H]+	7.92	224.08, 148.11
Dimethyl-phthalate	C10H10O4	Confirmed	195.0652 [M+H]+	5.75	163.04, 135.04, 84.96
Dinoseb	C10H12N2O5	Failed	239.0663 [M-H]-	11.9	194.05, 151.08
Diphenhydramine	C17H21NO	Confirmed	256.1701 [M+H]+	5.95	167.09, 152.06
Diuron	C9H10Cl2N2O	Failed	233.0243 [M+H]+	7.9	137.07, 94.07, 177.06
Dopamine	C8H11NO2	Failed	154.0868 [M+H]+	1.2	91.05, 119.05, 137.06

Emtricitabine	C8H10FN3O3S	Confirmed	248.0494 [M+H]+	2.2	130.04, 101.01, 73.01
Epinephrine	C9H13NO3	Failed	184.0968 [M+H]+	1.1	107.05, 166.09, 151.06
Estriol	C18H24O3	Failed	311.1618 [M+Na]+	5.85	208.88, 226.89, 190.87
Ethofumesate	C13H18O5S	Failed	287.0948 [M+H]+	8.9	121.06, 161.06, 137.06
Ethyl 3-(N-butylacetamido) propionate	C11H21NO3	Confirmed	216.1594 [M+H]+	6.6	128.11, 86.10
Famotidine	C8H15N7O2S3	Confirmed	338.0527 [M+H]+	2.3	189.03, 155.04, 71.06
Fenofibric Acid	C17H15ClO4	Confirmed	319.0732 [M+H]+	11.5	233.04, 138.99, 121.03
Fexofenadine	C32H39NO4	Confirmed	502.2958 [M+H]+	7.35	484.28, 466.27, 171.12
Fluconazole	C13H12F2N6O	Confirmed	307.1113 [M+H]+	4.5	220.067, 238.08, 169.05
Flucytosine	C4H4FN3O	Failed	130.0411 [M+H]+	1.1	113.01, 95.10, 87.04
Fluoxetine	C17H18F3NO	Confirmed	310.1413 [M+H]+	8.35	265.16, 105.03, 223.11
Fluridone	C19H14F3NO	Confirmed	330.1100 [M+H]+	8.45	310.10
Gabapentin	C9H17NO2	Confirmed	172.1332 [M+H]+	3.23	137.10, 154.12, 119.09
Gemfibrozil	C15H22O3	Confirmed	251.1642 [M+H]+	13.5	178.97, 208.98, 194.97
Gibberellic acid	C19H22O6	Failed	345.1333 [M-H]-	4.55	143.09, 221.13, 71.05
Haloperidol	C21H23ClFNO2	Failed	376.1490 [M+H]+	6.8	165.07, 123.03, 358.14
Hexazinone	C12H20N4O2	Failed	253.1659 [M+H]+	6.08	171.09, 71.06, 85.08

Hydrochlorothiazide	C7H8ClN3O4S2	Confirmed	297.9712 [M+H]+	2.33	232.98, 204.98, 280.95
Hydrocodone	C18H21NO3	Failed	300.1599 [M+H]+	2.84	199.08, 241.09
Hydrocortisone	C21H30O5	Failed	363.2171 [M+H]+	7	121.06, 97.06, 309.18
Ibuprofen	C13H18O2	Confirmed	229.1199 [M+Na]+	11.9	151.04, 101.06, 83.05
Indole-3-butyric acid (IBA)	C12H13NO2	Failed	204.1018 [M+H]+	6.8	130.07, 144.08, 168.08
Iodocarb	C8H12INO2	Confirmed	281.9985 [M+H]+	7.4	164.92, 57.07
Iohexol	C19H26I3N3O9	Confirmed	821.8881 [M+H]+	1.9	803.88, 602.91, 652.87
Irbesartan	C25H28N6O	Confirmed	429.2397 [M+H]+	7.9	207.09, 195.19
Irgarol	C11H19N5S	Confirmed	254.1434 [M+H]+	8.2	198.08, 91.03
Isoproturon	C12H18N2O	Failed	207.1491 [M+H]+	7.7	72.05, 134.10
Ketamine	C13H16ClNO	Confirmed	238.0998 [M+H]+	3.93	125.02, 179.06, 163.03
Ketoprofen	C16H14O3	Confirmed	255.1016 [M+H]+	8.45	105.03, 209.10, 177.05
Lacosamide	C13H18N2O3	Failed	251.1390 [M+H]+	4.45	91.05, 116.07, 74.06
Lamotrigine	C9H7Cl2N5	Confirmed	256.0151 [M+H]+	4.66	210.98
Levamisole	C11H12N2S	Confirmed	205.0794 [M+H]+	2.8	178.07, 129.07
Levetiracetam	C8H14N2O2	Confirmed	171.1123 [M+H]+	2.75	126.09, 69.03, 98.10
Levofloxacin	C18H20FN3O4	Confirmed	362.1516 [M+H]+	3.55	318.16, 261.10

Lidocaine	C14H22N2O	Confirmed	235.1805 [M+H]+	3.7	86.10
Linezolid	C16H20FN3O4	Failed	338.1516 [M+H]+	4.8	296.14, 235.12, 195.09
Losartan	C22H23ClN6O	Confirmed	423.1695 [M+H]+	7.9	207.09, 235.10, 171.07
Malaoxon	C10H19O7PS	Failed	315.0667 [M+H]+	6.2	99.01, 127.04, 142.99
Mecoprop	C10H11ClO3	Confirmed	213.0324 [M-H]-	9.7	141.01
Melamine	C3H6N6	Confirmed	127.0727 [M+H]+	1.1	85.05, 68.03, 110.05
Meprobamate	C9H18N2O4	Failed	219.1345 [M+H]+	5.4	97.10, 55.06, 69.07
Metalaxyl	C15H21NO4	Confirmed	280.1543 [M+H]+	7.6	160.11, 192.14, 220.13
Metaxalone	C12H15NO3	Confirmed	222.1125 [M+H]+	7.05	133.10, 105.07, 161.10
Metformin	C4H11N5	Confirmed	130.1087 [M+H]+	1.1	71.06, 60.06, 85.05
Methadone	C21H27NO	Confirmed	310.2165 [M+H]+	7.45	105.03, 265.16, 223.11
Methocarbamol	C11H15NO5	Confirmed	242.1028 [M+H]+	4.7	118.05, 163.08, 62.02
Metolachlor	C15H22ClNO2	Confirmed	284.1412 [M+H]+	10.5	252.11, 176.14
Metolachlor ESA	C15H23NO5S	Confirmed	330.1370 [M+H]+	6.65	298.11, 202.12, 160.11
Metoprolol	C15H25NO3	Confirmed	268.1907 [M+H]+	4.5	191.11, 159.08, 116.11
Metronidazole	C6H9N3O3	Confirmed	172.0722 [M+H]+	2.3	128.05, 98.05
Morphine	C17H19NO3	Confirmed	286.1438 [M+H]+	1.56	201.09, 229.09

N,N-Didesmethyl-venlafaxine	C15H23NO2	Failed	250.1802 [M+H]+	5.52	121.06, 147.08, 215.14
N4-acetylsulfadiazine	C12H12N4O3S	Failed	293.0703 [M+H]+	3.2	134.06, 198.02, 108.04
N4-Acetylsulfamethoxazole	C12H13N3O4S	Confirmed	296.0701 [M+H]+	4.8	134.06, 198.02, 108.04
Nadolol	C17H27NO4	Confirmed	310.2013 [M+H]+	3.55	254.14, 201.09, 236.13
Naproxen	C14H14O3	Confirmed	231.1016 [M+H]+	9	175.06, 185.10, 170.07
Nicotine	C10H14N2	Confirmed	163.1231 [M+H]+	1.11	130.07, 117.06
Norfloxacin	C16H18F1N3O3	Failed	320.1405 [M+H]+	3.7	276.15, 233.11, 256.14
Ofloxacin	C18H20FN3O4	Confirmed	362.1511 [M+H]+	3.53	318.16, 261.10
Oxcarbazepine	C15H12N2O2	Confirmed	253.0972 [M+H]+	5.7	208.08, 180.08, 236.07
Paraxanthine	C7H8N4O2	Confirmed	181.0726 [M+H]+	2.8	96.06, 124.05, 84.96
Penciclovir	C10H15N5O3	Failed	254.1248 [M+H]+	1.32	152.06, 67.05
Pentachlorophenol (PCP)	C6HCl5O	Failed	262.8392 [M-H]-	14.4	92.93
Pentobarbital	C11H18N2O3	Confirmed	227.1395 [M+H]+	2.03	70.07, 130.09
Pentoxifylline	C13H18N4O3	Confirmed	279.1457 [M+H]+	4.7	181.07, 138.07, 99.08
Perfluorobutyric acid (PFBA)	C4HF7O2	Confirmed	212.9792 [M-H]-	4.5	168.99
Perfluorooctanoic acid (PFOA)	C8HF15O2	Confirmed	412.9664 [M-H]-	11.2	168.99, 118.99
Phenobarbital	C12H12N2O3	Failed	231.077 [M-H]-	5.25	111.08, 156.95, 140.96

Phenylephrine	C9H13NO2	Failed	168.1025 [M+H]+	1.35	91.05, 109.06, 135.07
Phenytoin	C15H12N2O2	Failed	253.0977 [M+H]+	6.5	182.10, 104.05
Pirimicarb	C11H18N4O2	Failed	239.1503 [M+H]+	4.1	72.04, 137.07, 182.13
Primidone	C12H14N2O2	Failed	219.1128 [M+H]+	4.6	91.05, 162.09, 119.09
Progesterone	C21H30O2	Failed	315.2324 [M+H]+	11.6	109.06, 97.07, 170.07
Prometon	C10H19N5O	Confirmed	226.1662 [M+H]+	5.8	142.07, 184.12, 100.05
Propachlor ESA	C11H15NO4S	Failed	256.0649 [M-H]-	4.7	120.96, 79.96, 134.10
Propachlor OXA	C11H13NO3	Failed	208.0968 [M+H]+	4.8	120.04, 92.05
Propoxur	C11H15NO3	Failed	210.1125 [M+H]+	6	111.04, 93.03, 65.04
Propranolol	C16H21NO2	Confirmed	260.1651 [M+H]+	5.9	116.11, 183.08, 155.09
Pseudoephedrine	C10H15NO	Confirmed	166.1229 [M+H]+	2.8	133.09, 148.11, 117.07
Ranitidine	C13H22N4O3S	Confirmed	315.1485 [M+H]+	2.2	176.05, 130.06, 98.08
Ritalinic acid	C13H17NO2	Confirmed	220.1332 [M+H]+	4.05	84.08, 174.13
Saccharin	C7H5NO3S	Confirmed	181.9912 [M-H]-	2.55	105.96, 61.97
Sertraline	C17H17Cl2N	Failed	306.0816 [M+H]+	8.9	158.98, 129.07, 121.06
Siduron	C14H20N2O	Confirmed	233.1653 [M+H]+	8.9	137.07, 94.07, 120.04
Simazine	C7H12ClN5	Confirmed	202.0854 [M+H]+	6	132.03, 96.06, 124.09

Sitagliptin	C16H15F6N5O	Failed	408.1254 [M+H]+	4.55	235.08, 174.05, 193.07
Sotalol	C12H20N2O3S	Confirmed	273.1267 [M+H]+	2	133.08, 176.13, 213.07
Sucralose	C12H19Cl3O8	Confirmed	441.0128 [M-FA]-	3.9	165.02, 121.03
Sulfadiazine	C10H10N4O2S	Failed	251.0602 [M+H]+	2.35	156.01, 108.04, 96.06
Sulfamethazine	C12H14N4O2S	Failed	279.0910 [M+H]+	3.3	204.04, 124.09, 156.01
Sulfamethoxazole	C10H11N3O3S	Confirmed	254.0594 [M+H]+	3.9	237.09, 156.01, 108.04
Temazepam	C16H13ClN2O2	Confirmed	301.0744 [M+H]+	8.11	255.07, 228.06
Theophyline	C7H8N4O2	Confirmed	181.0725 [M+H]+	3	124.05, 96.06, 84.96
Thiabendazole	C10H7N3S	Failed	202.0433 [M+H]+	3.45	175.03, 131.06
Tramadol	C16H25NO2	Confirmed	264.1958 [M+H]+	4.2	58.07
Triamterene	C12H11N7	Confirmed	254.1154 [M+H]+	4	237.09, 156.01, 108.04
Tributyl phosphate	C12H27O4P	Confirmed	267.1725 [M+H]+	13.1	98.98
Triclocarban	C13H9Cl3N2O	Confirmed	314.9858 [M+H]+	13.35	161.99, 128.03, 93.06
Triclosan	C12H7Cl3O2	Confirmed	286.9428 [M-H]-	13.5	97.00, 115.92
Trimethoprim	C14H18N4O3	Confirmed	291.1452 [M+H]+	3.4	245.10, 123.07, 261.10
Trinexapac-ethyl	C13H16O5	Failed	253.1071 [M+H]+	7.9	69.03, 139.04, 165.02
Tris(1,3-dichloro-2-propyl)phosphate (TDCPP)	C9H15Cl6O4P	Confirmed	428.8917 [M+H]+	11.9	98.98, 208.95, 75.00

Tris(2-chloro-ethyl) phosphate	C6H12Cl3O4P	Confirmed	284.9611 [M+H]+	6.3	182.10, 98.98, 125.00
Valsartan	C24H29N5O3	Confirmed	436.2343 [M+H]+	9.7	235.10, 291.19, 207.09
Venlafaxine	C17H27NO2	Confirmed	278.2115 [M+H]+	5.5	121.06, 147.08, 58.07

[a]Accurate mass is the mass measured by the quadrupole-orbitrap mass spectrometer.

[b]The $[M+Na]^+$ adduct was identified as the most intense adduct for estriol and ibuprofen during compound tuning and was therefore used for sample screening.