



Screening of Emerging Contaminants in Water by HRAM MS

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WATER CONTAMINATION



Water Contamination Media and Public Awareness

More health news ... MBC NEWS.com

Pharmaceuticals lurking in U.S. drinking water

AP probe found traces of meds in water supplies of 41 million Americans

Energy and Environment

The Washington Post

Pesticides are polluting our waters – and we often don't know it

Fracking Chemicals Detected in Pennsylvania Drinking Water

By NICHOLAS ST. FLEUR MAY 4, 2015

The New York Times

Fears About Water Supply Grip Village That Made Teflon Products

64th ASMS WOC-410 June 8, 2016

Water Contaminants





Pain Points for Analysis



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Sample Analysis - Workflow



Automated Solid Phase Extraction Flexcube



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Method Parameters Flexcube + LC



Method Parameters 6550 QTOF-MS



Condition
Agilent 6550 Accurate-Mass QToF-MS with iFunnel technology
Positive electrospray ionization with dual jet stream
2 GHz extended dynamic range
Classic tune (m/z: 50-1700)
m/z: 50-1000
130 °C
16 L/min
375 °C
11 L/min
35 psi
365 V
3500



- 5-10x increase in ions sampled
- Enhanced sensitivity



Confidentiality Label 19 August 2016

Analysis of Emerging Compounds Traditional MS/MS



Analysis of Emerging Compounds All Ions MS/MS



Analysis of Emerging Compounds All Ions MS/MS Data Acquisition



Three Collision energy experiments performed simultaneously at 0, 10 & 40 eV □ Spectral acquisition at 4.5 spectra/sec



Confidentiality Label 19 August 2016

All Ions MS/MS Workflow – Find By Formula

sconng	Results		Result Filte	rs l	Frage	ment Confirmation
A Formula Sou	arce [Formula Match	hing	Positiv	e lons	Negative Ions
ource of formula These formula	s to confirm is:					
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Compound ex	change hie (,L	£F <u></u>				
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	S/N ratio	>=	9100]	
	Coelution score	>=	90]	
	Fragment ion confi	mation (criteria		
	Minimum num	ber of q	ualified fragments	1	
	Minimum perc	ent of a	valified fragments	75	



Water Screening PCDL Covering All Major Environmental Regulations





Analysis of Emerging Contaminants Personal Compound Database and Library (PCDL)

MassHunter PCDL Manager for Forensi	ics and Toxicology - C:\Mass	Hunter\PCDL\VetD	Drugs_AM_P	CDL.cdb					Ē		
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ectra for compound: Sun ametrizoie		TAR DEC	1982-938	13202.36	1.6 (5 56		50-				
Compound Name	Ion Species	Precursor Ion	CE (V)	Polarity	lonization		40-				
Sulfamethizole	(M+H)+	271.03179	9 10	Positive	ESI		20				
Sulfamethizole	(M+H)+	271.03179	9 20	Positive	ESI		108.04	305			
Sulfamethizole	(M+H)+	2/1.031/9	9 40	Positive	ESI		20- 15.5	9			
Sultamethizole	(M-H)-	269.01724	4 10	Negative	ESI	_	10-				
Sulfamethizala	(M-H)-	269.01724	4 20	Negative	ESI	Sec.		120 140 160 180 200	220 240	260	280
Suramethizole	(101-11)-	203.01724	4 40	Inegative	EDI		m/z	120 140 100 100 200	220 240	200 1	200
Compound Name	Formula	Mass Ar	nion Cat	ion BT ((min) (CAS	ChemSpider	IUPAC Name		Spe	ectra
Acetazolamide	C4H6N4O3S2	221 98813			594	66-5	1909 N-(5-S	ulfamovl-1 3 4thiadiazol-2-vl)ace	etamide	6	100
Bufexamac	C12H17NO3	223.12084			243	38-72-4	2372 2-(4-Bu	utoxyphenyl)-N-hydroxyacetamid	le	6	
Nabumetone	C15H16O2	228.11503		[[7]]	429	24-53-8	4256 4-(6-M	ethoxy-2-naphthyl)-2-butanone		6	
Naproxen	C14H14O3	230.09429			222	204-53-1	<u>137720</u> (25)-2-	137720 (2S)-2-(6-Methoxy-2-naphthyl)propanoic ac		acid 6	
Nalidixic acid	C12H12N2O3	232.08479			389	-08-2	4268 1-Ethy	1-Ethyl-7-methyl-4-oxo-1,4-dihydro-1,8-naphthy		6	
Methazolamide	C5H8N4O3S2	236.00378			554	1-57-4	3958 N-[(2Z)-3-Methyl-5-sulfamoyl-1,3,4-thiad	diazol-2(3H	. 6	
Amino-mebendazole	C14H11N3O	237.09021		(m)	523	329-60-9	36839 (2-amir	no-1H-benzimidazol-6-yl)(phenyl)	methanone	6	
Salbutamol (Albuterol)	C13H21NO3	239.15214			185	<u>59-94-9</u>	1999 2-(Hyd	roxymethyl)- <mark>4</mark> -{1-hydroxy-2-[(2-m	ethyl-2-pro	6	
Mefenamic acid	C15H15NO2	241.11028			<u>61-</u>	<u>68-7</u>	<u>3904</u> 2-[(2,3	-Dimethylphenyl)amino]benzoic a	acid	6	
Oxibendazole	C12H15N3O3	249.11134		1	205	59-55-1	4461 Methy	(5-propoxy-1H-benzimidazol-2-y	()carbamate	6	



Analysis of Veterinary Drugs in Meat All Ions MS/MS Method Conditions





Precursor Identification

•Mass Tolerance: 10 ppm •Retention Time Tolerance: 0.2 min

Minimum Absolute Area Counts: 10.000





Fragment Confirmation

Min. Number of fragments req.: 1 Minimum S/N: 9.0 Coelution score: >90.0



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Compour	nd List			Results: Cpd 69: Mekwicam ×
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	E Cod CO Mideuro	P141/10.N0.04.02		ID Techniques Applied 4
	9 End 32: Sulfachloropuridazing	Dualified C10 H9 CIN4 02 S	97.74 294.0142	
	7 Cpd 78: Eproflovacin	Qualified C10 H3CI N4 02 5	96.21 359.1654	Best = Name = Formula = m/z / = Mass = Mass (Tgt) = Diff(ppm) = Score(Tgt) = RT == RT (Tgt) = RT Diff = Score(RT
	6 Cod 29: Sulfadimidine (Sulfamethazine)	Qualified C12 H14 N4 O2 S	96.52 278.0844	Image: Meloxicam C14 H13 N3 04 S2 352.0429 374.0244 351.0356 351.0347 -2.32 95.07 7.146 7.0 3 0.123
3	7 Cpd 26: Sulfamerazine	Qualified C11 H12 N4 O2 S	97.34 264.0688	Coelution Score + CE + Flags(Fls) + FV + Height + m/z + Compound Name + RT + RT Diff + SNR +
	6 Cpd 45: Flunixin-d3	Qualified C14 H8 D3 F3 N2	97.88 299.0969	97.9 10 Qualified 289858.4 115.0324 Meloxicam 7.14 0.006 248
1-	4 Cpd 23: <tolfenamic acid=""></tolfenamic>	Not qualified C14 H12 CI N O2	95.91 261.0563	98.3 40 Qualified 84489.2 141.0117 Meloxicam 7.14 0.006 261.6
0-	4 Cpd 6: <hydroxy-ipronidazole></hydroxy-ipronidazole>	Not qualified C7 H11 N3 O3	94.9 185.0805	- 62.5 Low coelution score 4855.7 184.0539 Meloxicam 7.14 0.006 14
9-	6 Cpd 35: Sulfaethoxypyridazine	Qualified C12 H14 N4 O3 S	98.95 294.0795	EIC with zero abund 73.0106 Meloxicam
) and the second se	4 Cpd 38: Flunixin	Qualified C14 H11 F3 N2 O2	83.94 296.0781	Low S/N ratio 4910.1 153.0005 Meloxicam 7.14 5.4
< <u> </u>	Cod 43: Fenhendezole	Ouslified C15 H12 N2 O2 S	95.1 299.0727	III
Compour	nd Chromatogram Besults			X Ci) Compound Fragment Spectrum Results
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3- 2.5- 2- 1.5- 1- 0.5-		X146 213304	213 + 213 +	cps2.0420.374.024 x10 5 Cpd 69: Meloxicam: +ESI HighE Scan (it: 7.092-7.223 min, 24 scans) B-Liver 1x.d AvgCE c-Frag(141.0117) Scan 2- 123.0920 c-Frag(141.0117) Scan 2- 2- c-Frag(153.0005) Scan 2- 2-
Ť	7.04 7.05 7.06 7.07 7.08 7.09 7.1 7.11 7.1	2 7.13 7.14 7.15 7.16 7.17 7.18 7.19 7.2 Counts vs. Acquisition Time (min)	21 7.22 7.23 7.24 7.25 7.26 7	
10 5- 1 0.5- 0.1			++E	EIC-Frag(115.0324) EIC-Frag(141.0117) I.4- 1.2- 1- 0.8- 0.6-
	7.04 7.05 7.06 7.07 7.08 7.09 7.1 7.11 7.	2 7.13 7.14 7.15 7.16 7.17 7.18 7.19 7.2	7.21 7.22 7.23 7.24 7.25 7.26 7 min)	7.27 7.28 7.29 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300 310 320 330 340 350 360
	ha	io magnetic fonzetecuisor fon vs. Acquisition Time	11011)	



Sampling Locations



Mill Creek (1-4) and Corey Creek (5) are tributaries of the Tioga River (7) which discharges into the Susquehanna River. The River serves as a source of drinking water to 4.1 million people in NY, PA and MD.

SAMPLE COLLECTION

40 mL samples collected in amber glass vials and shipped to the lab on ice within 24 hours.

Statistical Differentiation of Samples Mass Profiler Professional







64th ASMS WOC-410

23

PCA Scores Plot



Tukeys HSD 746 Entities Location 6 vs Controls



115 Compounds in Wastewater that are absent upstream



•

Database Search of Location 6 Only Entity List (115)

Cpd	74		Label 🛛 🖓 -	■ Name ⊽⊽⊀	P Formula ⊽+P	Score ⊽ +	Mass ⊽ +Þ	RT 🖓 🖶
	38		Cpd 38: Valethamat; C19 H32 N O2; 9.27	3 Valethama	t C19 H32 N O2	99.86	306.2436	9.273
	63	Cpd 63	trans-10,11-Dihydroxy-10,11-dihydroca	. trans-10,11-Dihydroxy-10,11-dihydro.	C15 H14 N2 O3	53.99	270.0956	8.167
	56	Сро	56: Sulmepride; C14 H21 N3 O4 S; 7.74	9 Sulmepride	C14 H21 N3 O4 S	87.87	327.1231	7.749
	66		Cpd 66: Pyridarone; C13 H9 N O; 10.11	7 Pyridarone	C13 H9 N O	97.72	195.0693	10.117
2.52 17.2	78	C	od 78: Pipebuzone; C25 H32 N4 O2; 7.88	B Pipebuzone	C25 H32 N4 O2	72.96	420.2559	7.888
	65	Cpd 6	5: Oxcarbazepine; C15 H12 N2 O2; 9.00	0 Oxcarbazepine	C15 H12 N2 O2	65.54	252.0848	9
	26	(Cpd 26: Irbesartan; C25 H28 N6 O; 10.13	7 Irbesartar	C25 H28 N6 O	99.18	428.2329	10.137
	61	(Cpd 61: Fenretinide; C26 H33 N O2; 7.76	6 Fenretinide	e C26 H33 N O2	9.86	391.2311	7.766
		23	Cpd 23	Dehydroepiandros	sterone; C19	H28 C)2; 13	.367
Ĵ.		113	(Cpd 113: Carbamaz	epine; C15 H	112 N2	2 0; 9	.810
		34		Cpd 34: Cann	ogenin; C23	H32 C)5; 14	660
		1.0						
	43	Cr	d 43: Benderizine; C28 H34 N2 O2; 8.01	4 Benderizine	C28 H34 N2 O2	68.19	430.2665	8.014
	43 22	Cpd 22	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1	4 Benderizine 3-(4-methylbenzylidene)-Campho	C28 H34 N2 O2 C18 H22 O	68.19 58.54	430.2665 254.1662	8.014 14.274
	43 22 15	Cpd 22 Cpd 22	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1. od 15: 17 a-Estradiol; C18 H24 O2; 14.10	4 Benderizine 3-(4-methylbenzylidene)-Campho 0 17 a-Estradio	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2	68.19 58.54 96.94	430.2665 254.1662 272.1783	8.014 14.274 14.1
	43 22 15 17	Cpd 22 Cpd 22 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1 od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39	4 Benderizine 3-(4-methylbenzylidene)-Camphon 0 17 a-Estradio 0 17 a-Estradio	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2	68.19 58.54 96.94 85.62	430.2665 254.1662 272.1783 272.1785	8.014 14.274 14.1 12.39
	43 22 15 17 1	Cpd 22 Cpd 22 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1. od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60	4 Benderizine 3-(4-methylbenzylidene)-Camphol 0 17 a-Estradio 17 a-Estradio 2	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4	68.19 58.54 96.94 85.62 95.26	430.2665 254.1662 272.1783 272.1785 248.1733	8.014 14.274 14.1 12.39 11.602
	43 22 15 17 1 2	Cpd 2 Cpd 2 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1 od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60	4 Benderizine 3-(4-methylbenzylidene)-Camphon 0 17 a-Estradio 0 17 a-Estradio 2 3	C28 H34 N2 O2 C18 H22 O C18 H24 O2 C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2	68.19 58.54 96.94 85.62 95.26 93.34	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394	8.014 14.274 14.1 12.39 11.602 8.603
	43 22 15 17 1 2 3	Cpd 2 Cpd 2 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1 od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60 Cpd 3: C21 H31 N O2 S2; 9.64	4 Benderizine 3-(4-methylbenzylidene)-Camphol 0 17 a-Estradio 0 17 a-Estradio 2 3 0	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2 C21 H31 N O2 S2	68.19 58.54 96.94 85.62 95.26 93.34 87.13	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394 393.1802	8.014 14.274 14.1 12.39 11.602 8.603 9.64
	43 22 15 17 1 2 3 4	Crd 22 Cpd 22 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1. od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60 Cpd 3: C21 H31 N O2 S2; 9.64 Cpd 4: C18 H20 N; 13.41	4 Benderizine 3-(4-methylbenzylidene)-Camphon 0 17 a-Estradio 0 17 a-Estradio 2 3 0 7	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2 C21 H31 N O2 S2 C18 H20 N	68.19 58.54 96.94 85.62 95.26 93.34 87.13 83.16	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394 393.1802 250.1592	8.014 14.274 14.1 12.39 11.602 8.603 9.64 13.417
	43 22 15 17 1 2 3 4 5	Cpd 22 Cpd 22 Cp	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1 od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60 Cpd 3: C21 H31 N O2 S2; 9.64 Cpd 4: C18 H20 N; 13.41 Cpd 5: C16 H24 O2; 12.32	4 Benderizine 3-(4-methylbenzylidene)-Campho 17 a-Estradio 17 a-Estradio 2 3 0 7 9	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2 C21 H31 N O2 S2 C18 H20 N C16 H24 O2	68.19 58.54 96.94 85.62 95.26 93.34 87.13 83.16 96.9	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394 393.1802 250.1592 248.1786	8.014 14.274 14.1 12.39 11.602 8.603 9.64 13.417 12.329
	43 22 15 17 1 2 3 4 5 6	Cpd 22 Cpd 22 Cl	od 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1. od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60 Cpd 3: C21 H31 N O2 S2; 9.64 Cpd 4: C18 H20 N; 13.41 Cpd 5: C16 H24 O2; 12.32 Cpd 6: C10 H24 N3 O5; 12.63	4 Benderizine 3-(4-methylbenzylidene)-Camphol 0 17 a-Estradio 0 17 a-Estradio 2 3 0 7 9 5	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2 C21 H31 N O2 S2 C18 H20 N C16 H24 O2 C10 H24 N3 O5	68.19 58.54 96.94 85.62 95.26 93.34 87.13 83.16 96.9 83.74	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394 393.1802 250.1592 248.1786 266.1713	8.014 14.274 14.1 12.39 11.602 8.603 9.64 13.417 12.329 12.635
	43 22 15 17 1 2 3 4 5 6 7	Cpd 22 Cpd 22 Cl	d 43: Benderizine; C28 H34 N2 O2; 8.01 2: 3-(4-methylbenzylidene)-Camphor; C1. od 15: 17 a-Estradiol; C18 H24 O2; 14.10 od 17: 17 a-Estradiol; C18 H24 O2; 12.39 Cpd 1: C11 H24 N2 O4; 11.60 Cpd 2: C32 H17 N2; 8.60 Cpd 3: C21 H31 N O2 S2; 9.64 Cpd 4: C18 H20 N; 13.41 Cpd 5: C16 H24 O2; 12.32 Cpd 6: C10 H24 N3 O5; 12.63 Cpd 7: C9 H24 N4 O2 S; 12.03	4 Benderizine 3-(4-methylbenzylidene)-Camphol 0 17 a-Estradio 0 17 a-Estradio 2 3 0 7 9 5 6	C28 H34 N2 O2 C18 H22 O C18 H22 O C18 H24 O2 C18 H24 O2 C11 H24 N2 O4 C32 H17 N2 C21 H31 N O2 S2 C18 H20 N C16 H24 O2 C10 H24 N3 O5 C9 H24 N4 O2 S	68.19 58.54 96.94 85.62 95.26 93.34 87.13 83.16 96.9 83.74 72.88	430.2665 254.1662 272.1783 272.1785 248.1733 429.1394 393.1802 250.1592 248.1786 266.1713 252.1616	8.014 14.274 14.1 12.39 11.602 8.603 9.64 13.417 12.329 12.635 12.036

Identification of Unknowns- Data Independent Analysis

All Ions MS/MS

Coelution Score	₹-₽	CE +	Flags(Fls) 🕂	FV -	Height 🕂	m/z +₽	
	98.8	10	Qualified		4092627	194.0964	1
	98.6	40	Qualified		1973776.7	193.0886	Ī
	97.1	40	Qualified		1485877.2	192.0808	
	96.4	40	Qualified		972295.9	179,073	
	89.6		Low coelution score		633932.9	165.0699	



Carbamazepine

Sample Location 5



Sample Location 6



Pain Points for Analysis





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Analysis of Water Contaminants Summary

- The current LC-QTOF MS systems can offer rapid screening of several hundred emerging compounds in real water samples
- Online Automated SPE allows users to analyze samples rapidly and with very little water sample while maintaining sensitivity
- All lons MS/MS workflow allows for additional verification tools in suspect screening with fragment confirmation and retention time through personal compound database and libraries (PCDLs)
- Several contaminants are detected in water; statistical analysis to choose SIGNIFICANT ones are essential





For more information please visit: www.agilent.com/en-us/solutions/environmental

Speaker contact: tarun.anumol@agilent.com



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