

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
 Data File : VN070498.D
 Acq On : 5 Jan 2022 18:54
 Operator : JC/MD
 Sample : N1012-15
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31332

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070498.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.233	78	91	101	rBV2	284225	594834	10.82%	1.802%
2	3.687	617	633	670	rVB	180365	507628	9.23%	1.538%
3	4.290	836	858	865	rBV2	137965	343432	6.25%	1.040%
4	4.357	867	883	927	rVB	996578	2915404	53.02%	8.831%
5	7.072	1870	1895	1910	rBV4	28512	89089	1.62%	0.270%
6	7.281	1954	1973	1981	rBV2	26493	64708	1.18%	0.196%
7	7.340	1985	1995	2020	rVB2	42492	112148	2.04%	0.340%
8	7.691	2097	2126	2149	rBV4	46432	148590	2.70%	0.450%
9	8.021	2225	2249	2260	rBV2	672774	1623452	29.52%	4.918%
10	8.083	2261	2272	2298	rVB	1203304	2712871	49.33%	8.218%
11	8.437	2382	2404	2430	rBV	861684	1990148	36.19%	6.029%
12	8.836	2537	2553	2575	rBV2	25578	58991	1.07%	0.179%
13	8.968	2575	2602	2635	rBV	1835459	3848825	69.99%	11.659%
14	9.410	2752	2767	2784	rBV2	29226	63034	1.15%	0.191%
15	10.252	3063	3081	3096	rBV	64239	134095	2.44%	0.406%
16	10.330	3097	3110	3127	rVB2	49372	92429	1.68%	0.280%
17	10.440	3133	3151	3166	rBV	2926964	5499000	100.00%	16.658%
18	10.505	3166	3175	3203	rVB	300939	599606	10.90%	1.816%
19	11.744	3619	3637	3659	rBV	2440877	4419438	80.37%	13.387%
20	12.277	3824	3836	3854	rBV5	43670	108139	1.97%	0.328%
21	12.358	3856	3866	3885	rVB2	34783	74592	1.36%	0.226%
22	12.731	3989	4005	4033	rBV	2037415	3607592	65.60%	10.928%
23	13.675	4342	4357	4376	rBV	1845186	3207804	58.33%	9.717%
24	13.768	4384	4392	4408	rVB2	117379	196145	3.57%	0.594%

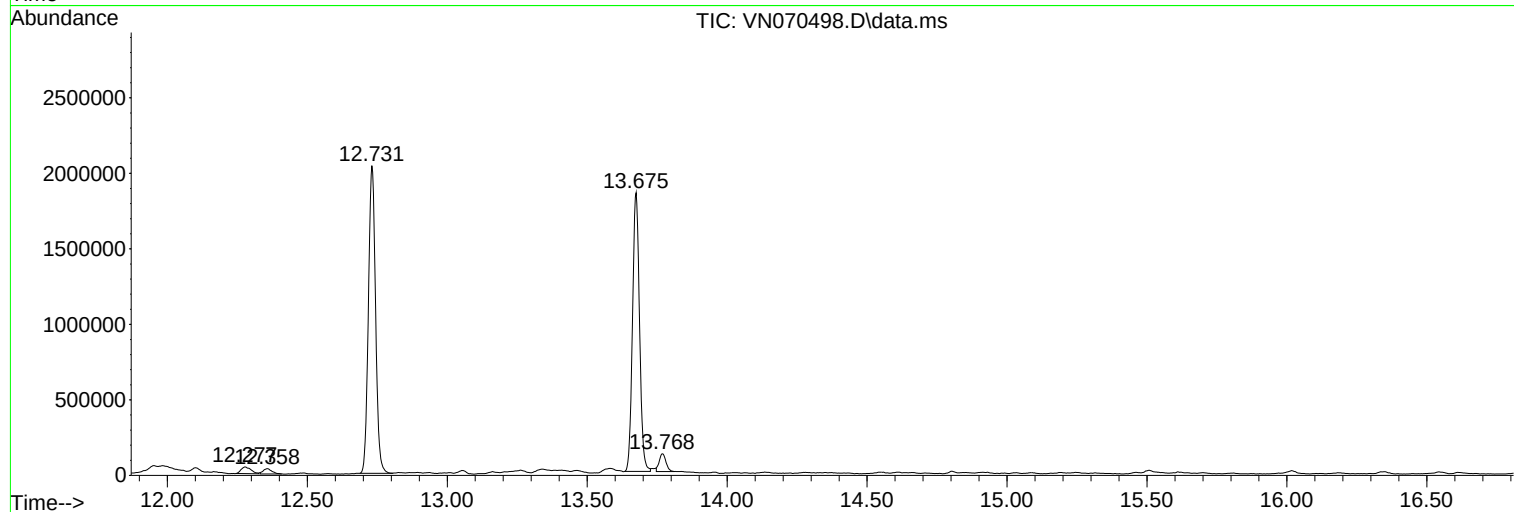
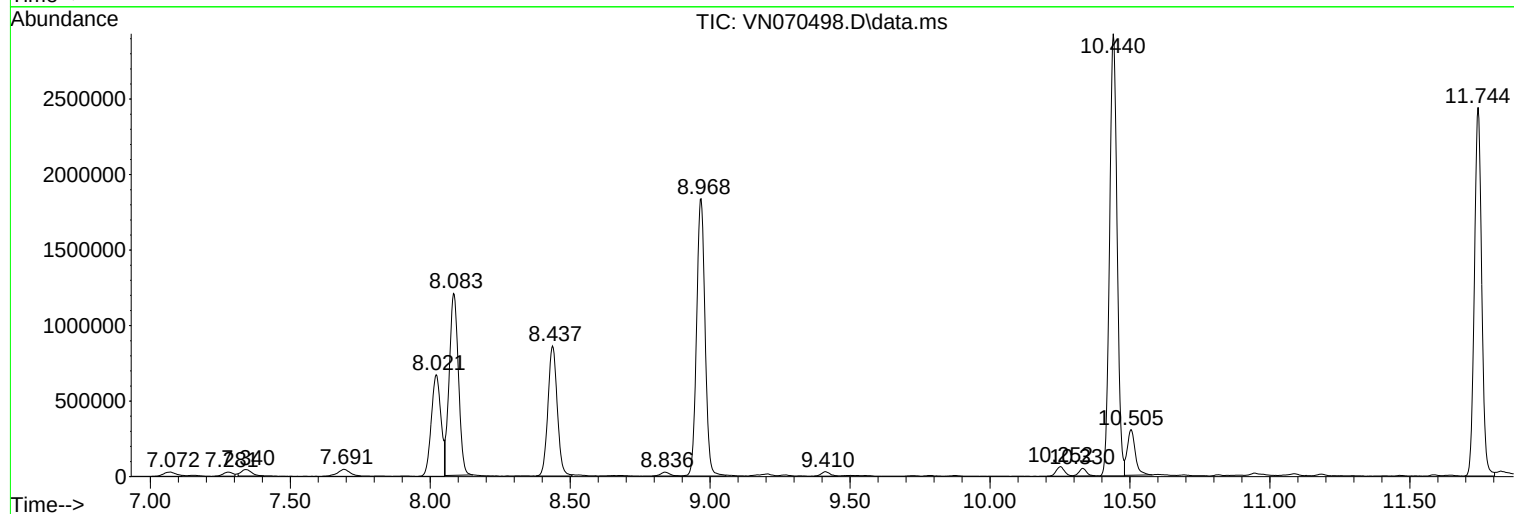
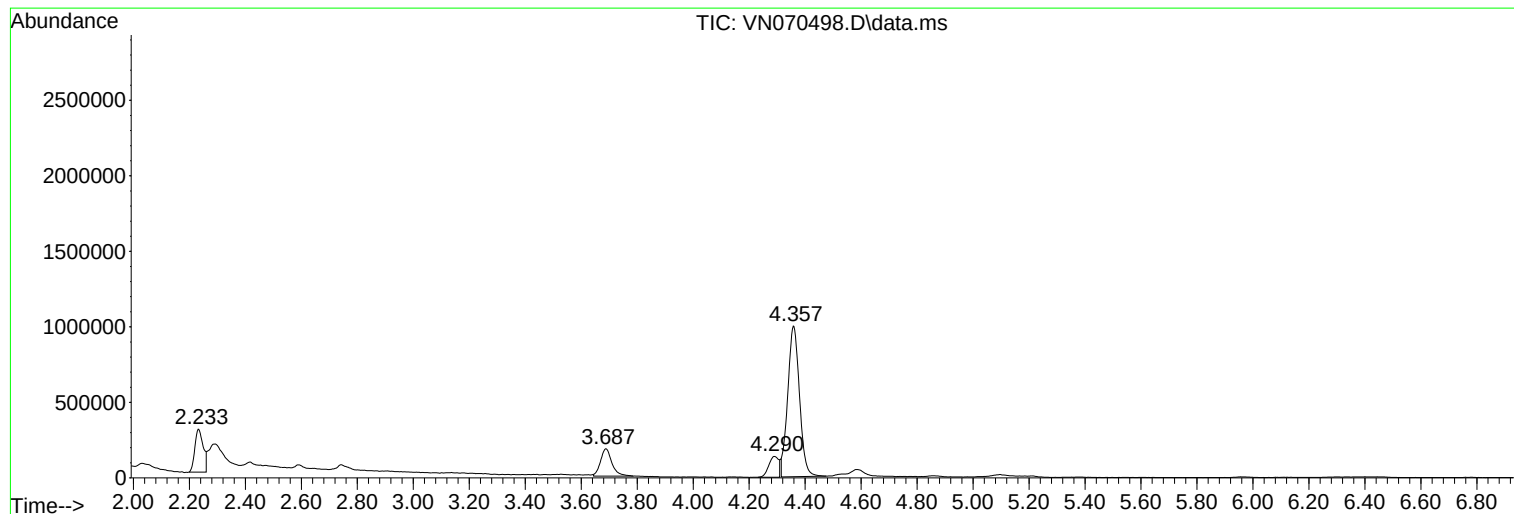
Sum of corrected areas: 33011994

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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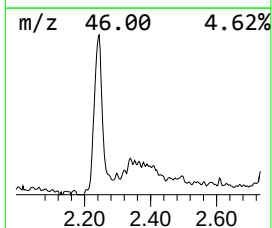
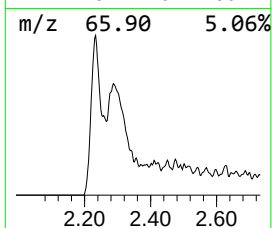
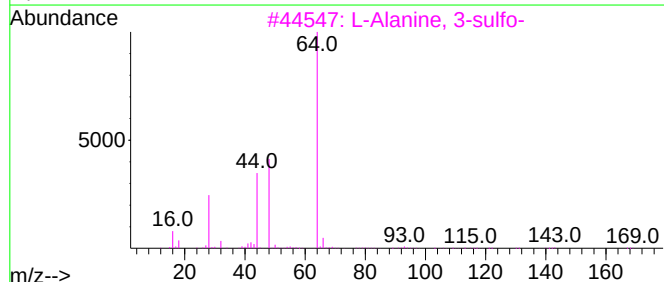
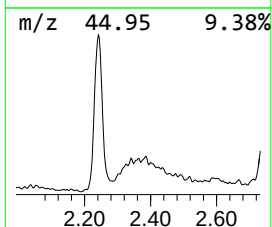
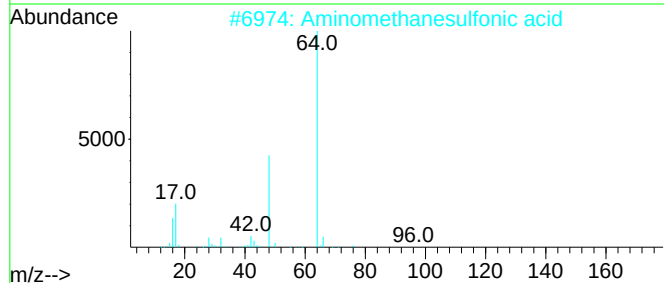
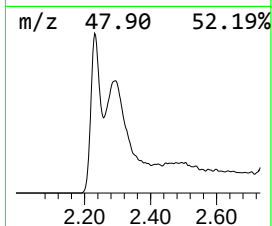
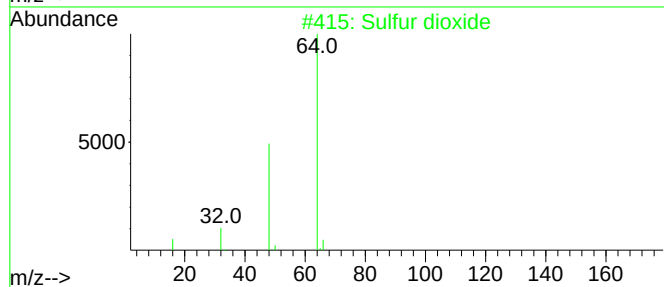
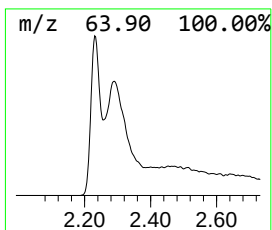
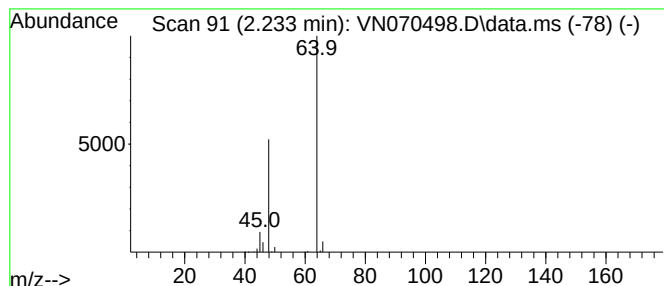
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.233	10.96 ug/l	594834	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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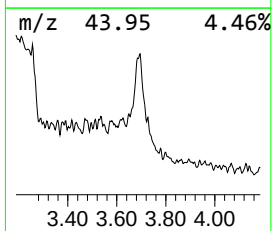
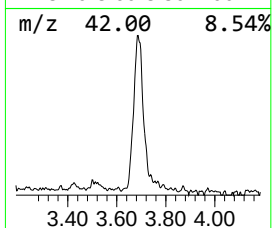
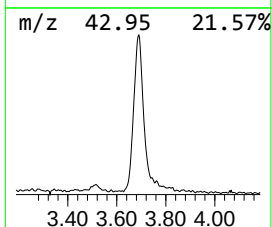
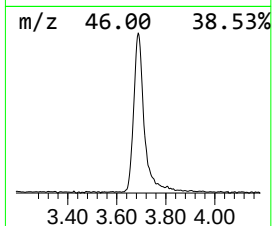
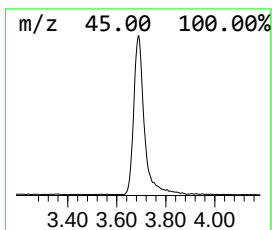
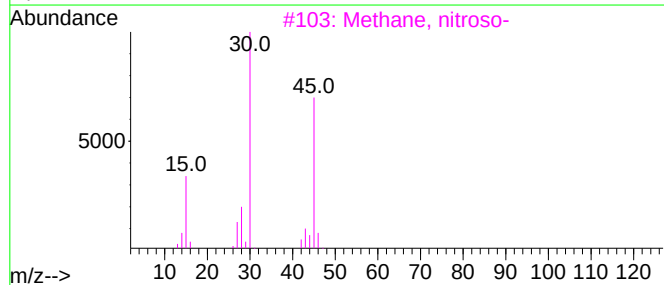
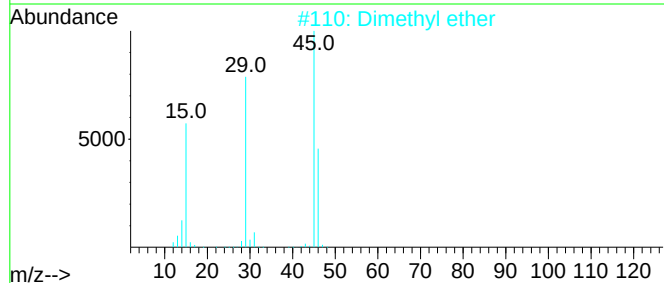
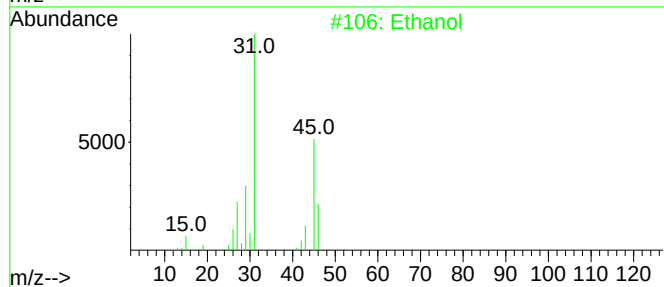
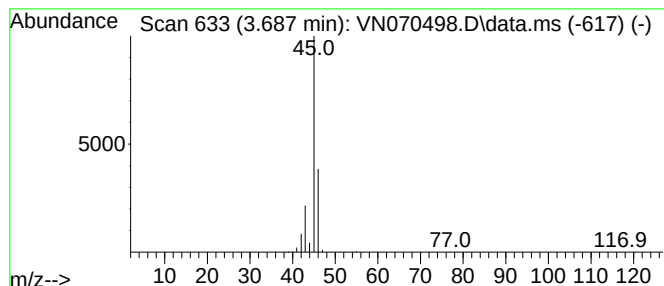
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.687	9.36 ug/l	507628	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol			46	C2H6O	000064-17-5	64
2	Dimethyl ether			46	C2H6O	000115-10-6	9
3	Methane, nitroso-			45	CH3NO	000865-40-7	4
4	Formic acid			46	CH2O2	000064-18-6	4
5	Formamide			45	CH3NO	000075-12-7	2



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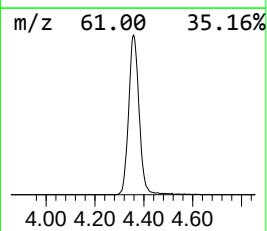
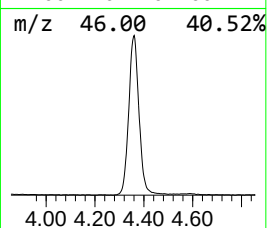
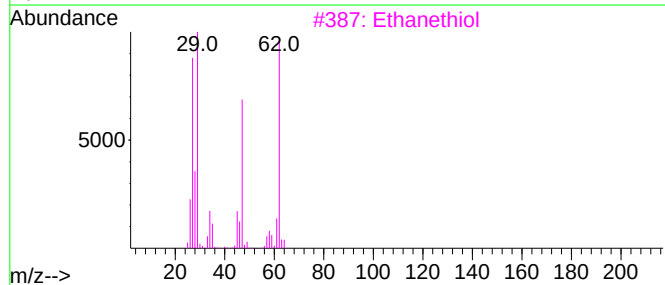
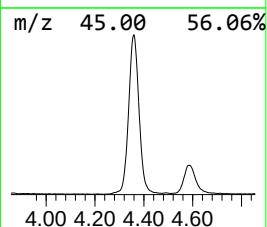
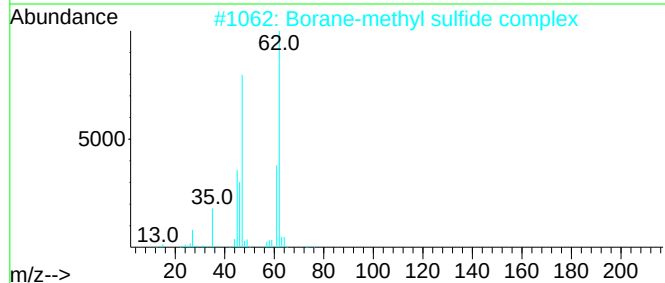
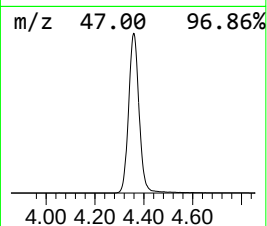
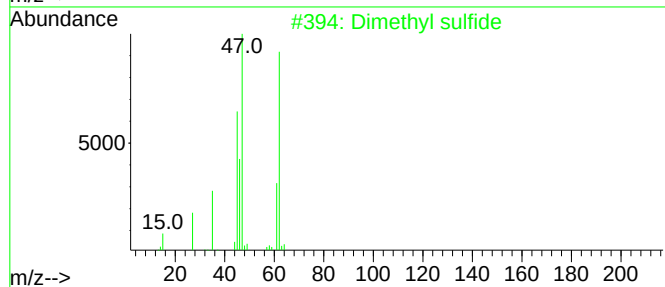
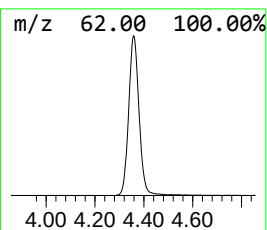
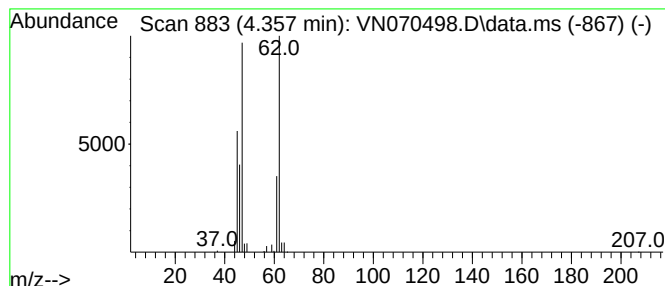
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.357	53.73 ug/l	2915400	Pentafluorobenzene	8.085

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5			Propane, 2-fluoro-	62	C3H7F	000420-26-8	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.233	11.0	ug/l	594834	1	8.085	2712870	50.0
Ethanol	3.687	9.4	ug/l	507628	1	8.085	2712870	50.0
Dimethyl sulfide	4.357	53.7	ug/l	2915400	1	8.085	2712870	50.0