

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010622\
 Data File : VN070518.D
 Acq On : 6 Jan 2022 14:46
 Operator : JC/MD
 Sample : N1012-08
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31240

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: VN070518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	77	92	150	rBV2	20756720	35627654	100.00%	60.254%
2	7.064	1866	1892	1920	rBV4	1753336	534237	1.50%	0.904%
3	8.021	2223	2249	2260	rBV	579765	1392836	3.91%	2.356%
4	8.083	2260	2272	2310	rVB	1016042	2347992	6.59%	3.971%
5	8.437	2383	2404	2433	rBV	731262	1717323	4.82%	2.904%
6	8.965	2581	2601	2627	rBV	1507029	3167445	8.89%	5.357%
7	10.440	3131	3151	3174	rBV	2473348	4612926	12.95%	7.802%
8	11.186	3410	3429	3472	rBV2	184417	465885	1.31%	0.788%
9	11.744	3614	3637	3665	rBV	1961665	3662562	10.28%	6.194%
10	12.731	3978	4005	4033	rBV	1680604	3067589	8.61%	5.188%
11	13.675	4340	4357	4382	rBV	1422395	2532183	7.11%	4.282%

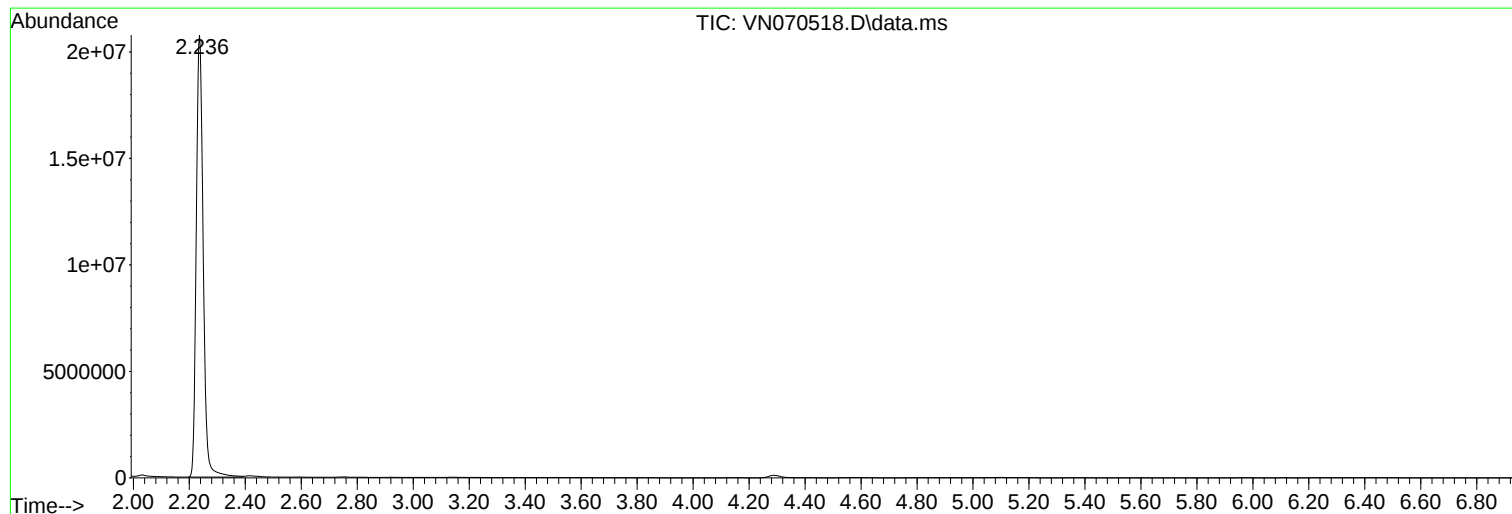
Sum of corrected areas: 59128632

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Quant Title : SW846 8260

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



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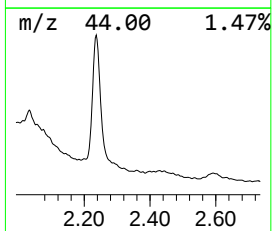
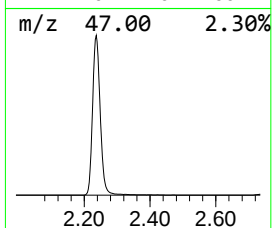
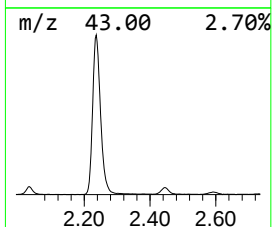
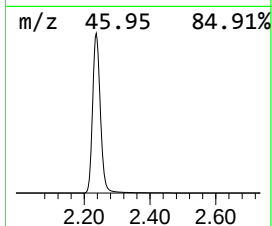
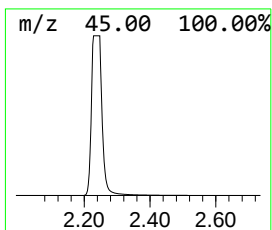
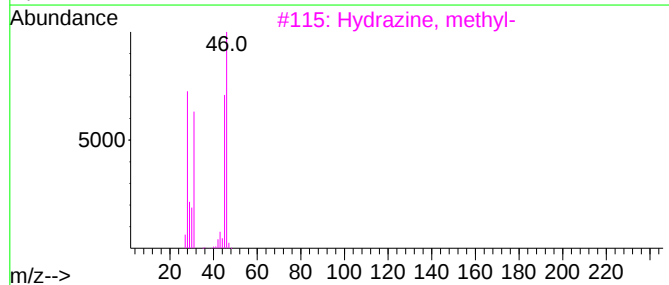
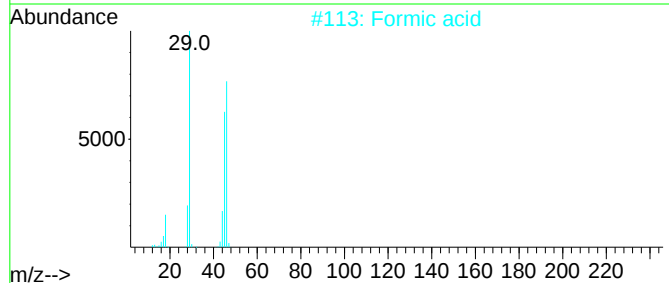
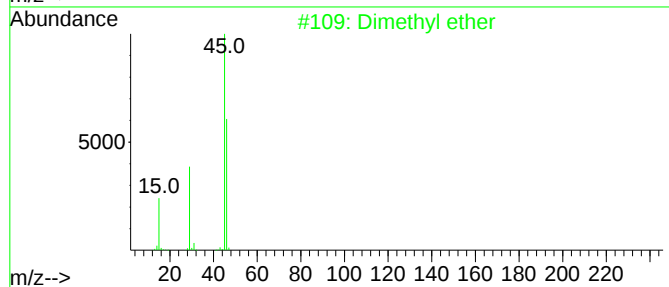
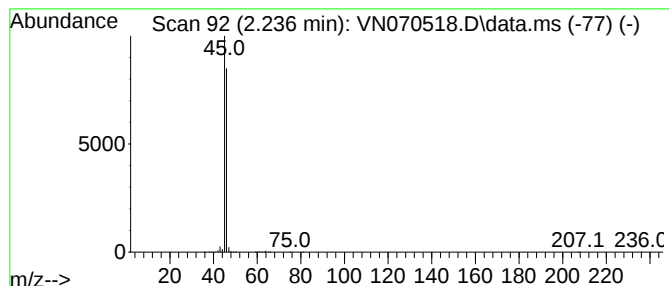
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.236 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.236	758.68 ug/l	35627700	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl ether	46	C2H6O	000115-10-6	9
2			Formic acid	46	CH2O2	000064-18-6	7
3			Hydrazine, methyl-	46	CH6N2	000060-34-4	4
4			Ethene, fluoro-	46	C2H3F	000075-02-5	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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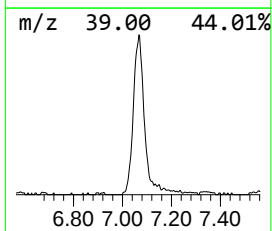
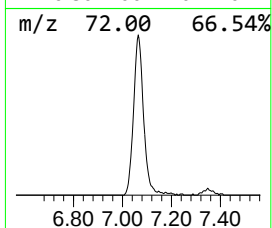
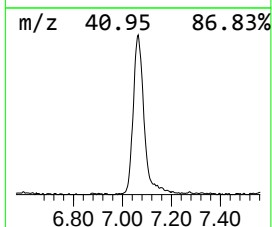
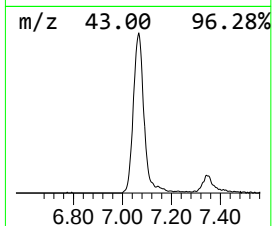
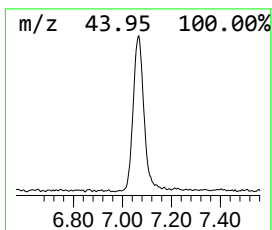
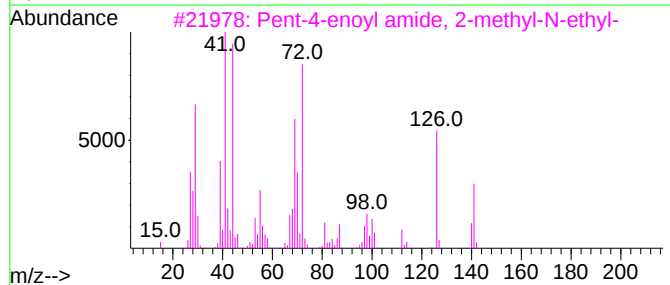
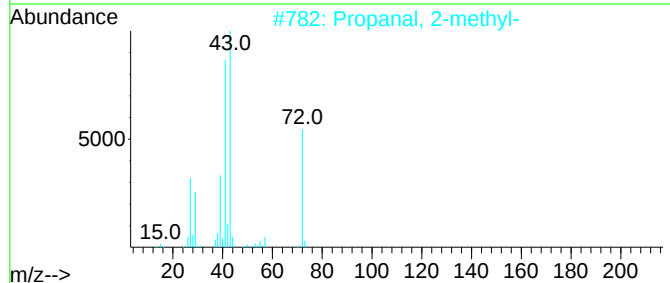
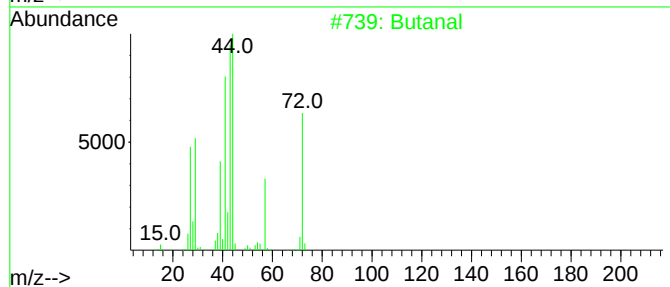
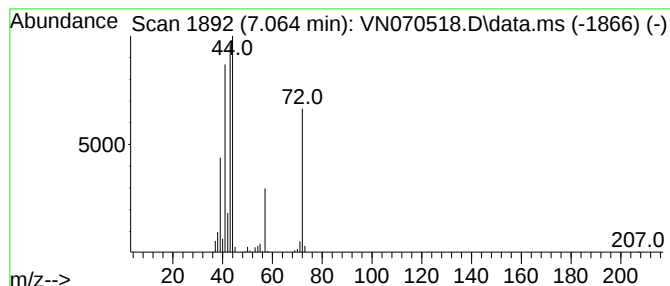
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Peak Number 2 Butanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.064	11.38 ug/l	534237	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Propanal, 2-methyl-	72	C4H8O	000078-84-2	52
3			Pent-4-enoyl amide, 2-methyl-N-e...	141	C8H15NO	1000420-35-1	45
4			Ethene, ethoxy-	72	C4H8O	000109-92-2	40
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	32



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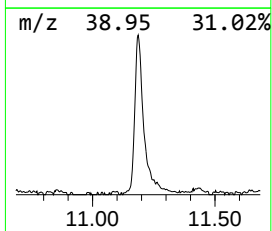
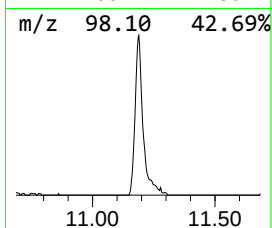
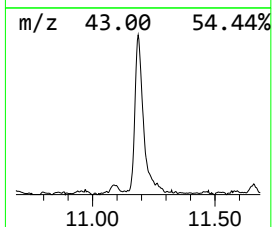
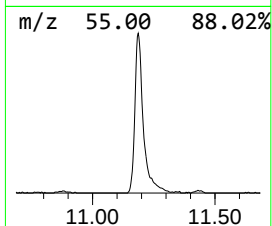
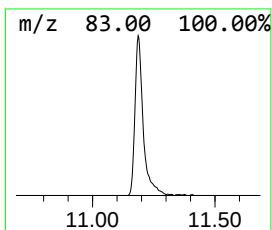
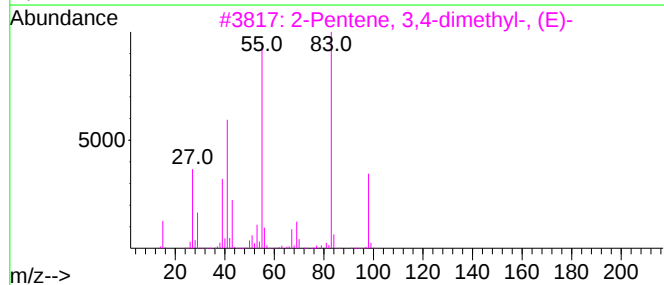
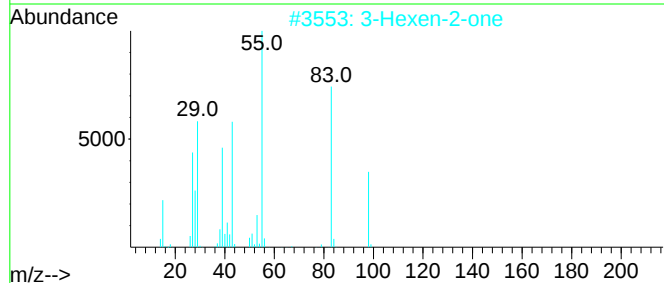
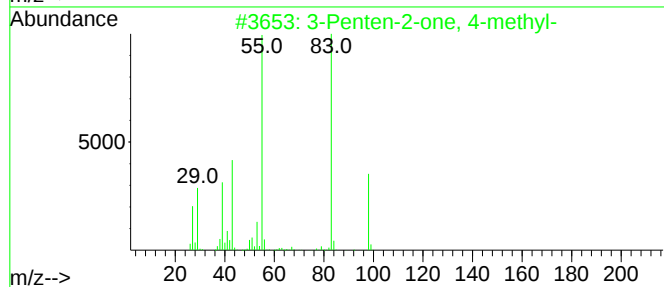
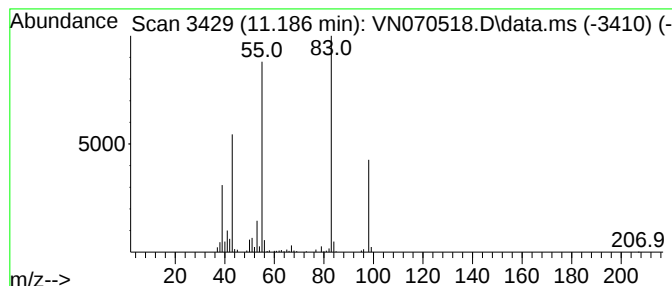
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Peak Number 3 3-Penten-2-one, 4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.186	6.36 ug/l	465885	Chlorobenzene-d5	11.744

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
2			3-Hexen-2-one	98	C6H10O	000763-93-9	91
3			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	86
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80
5			2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown2.236	2.236	758.7	ug/l	35627700	1	8.086	2347990	50.0
Butanal	7.064	11.4	ug/l	534237	1	8.086	2347990	50.0
3-Penten-2-one,...	11.186	6.4	ug/l	465885	3	11.744	3662560	50.0