

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
 Data File : VN068492.D
 Acq On : 15 Sep 2021 18:40
 Operator : JC/MD
 Sample : M3759-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31207

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\82N090721W.M

Title : SW846 8260

Signal : TIC: VN068492.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.518	191	197	264	rBV2	46850972	205275095	100.00%	65.369%
2	4.055	764	770	771	rBV3	48587946	31718296	15.45%	10.100%
3	6.624	1689	1728	1776	rVB	9345687	32320029	15.74%	10.292%
4	7.061	1863	1891	1918	rBV	1666309	4624027	2.25%	1.472%
5	8.086	2260	2273	2298	rVB	1344926	3028617	1.48%	0.964%
6	8.968	2586	2602	2633	rVB	1605269	3323007	1.62%	1.058%
7	10.443	3134	3152	3166	rBV2	2747771	5594170	2.73%	1.781%
8	11.223	3430	3443	3458	rVB	1511351	2739472	1.33%	0.872%
9	11.714	3612	3626	3635	rBV2	3713094	7750191	3.78%	2.468%
10	12.733	3997	4006	4034	rVB	1446713	2714656	1.32%	0.864%
11	13.525	4288	4301	4315	rBV	1363725	2194551	1.07%	0.699%
12	13.675	4343	4357	4376	rVB	1612665	2821256	1.37%	0.898%
13	14.522	4660	4673	4688	rVB	1867693	2924720	1.42%	0.931%
14	15.024	4846	4860	4876	rBV	2085294	3308502	1.61%	1.054%
15	15.158	4898	4910	4938	rVB	2234142	3690475	1.80%	1.175%

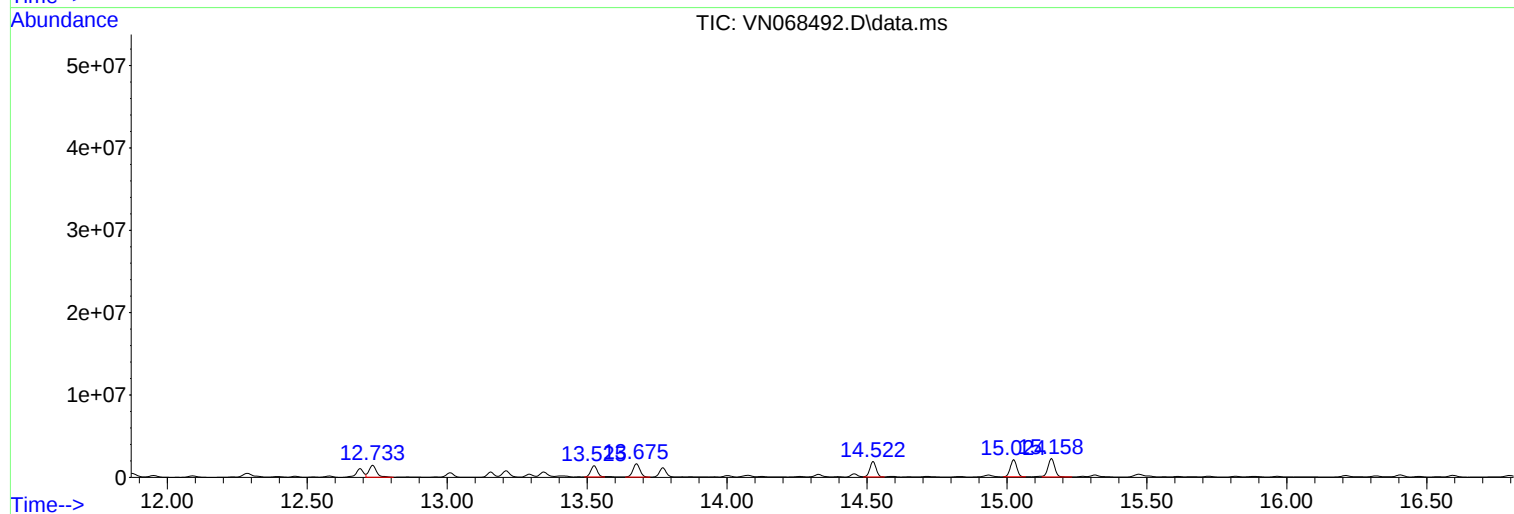
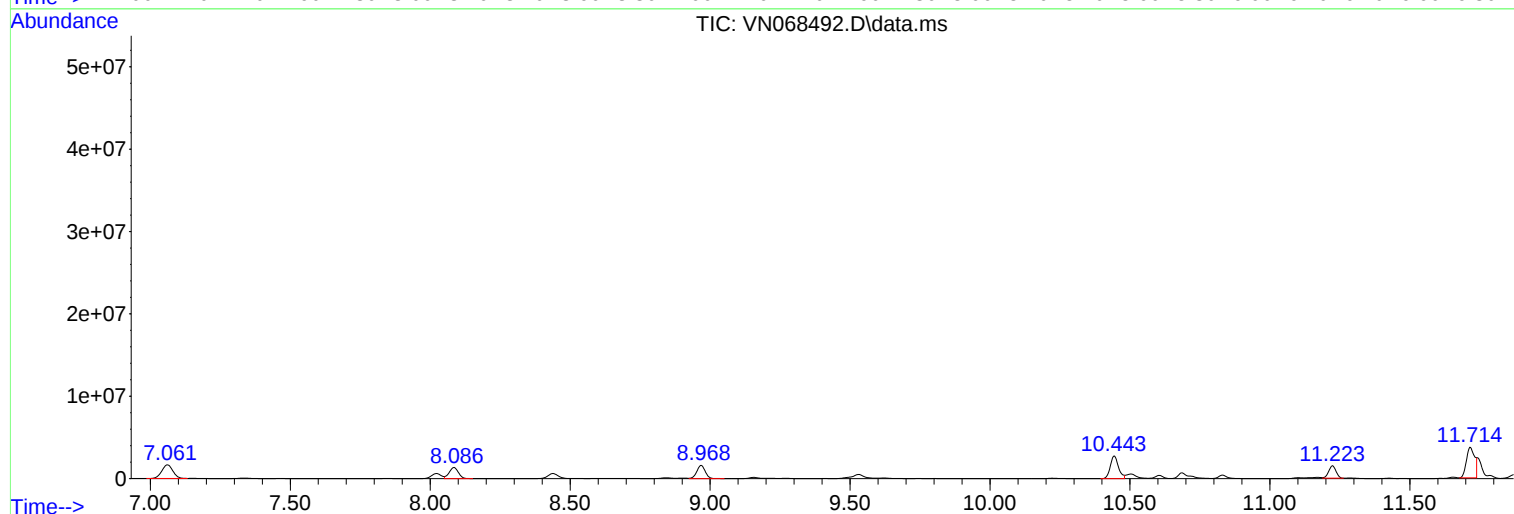
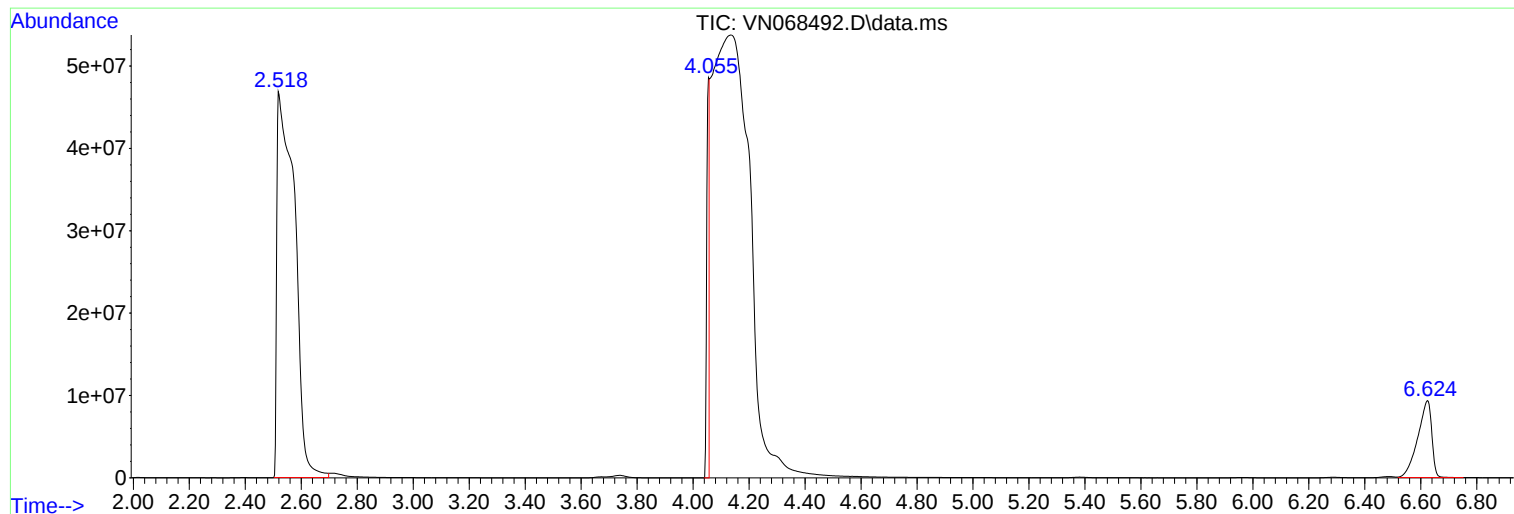
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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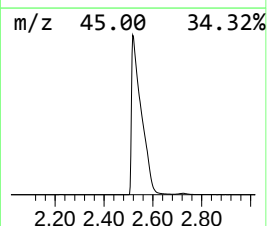
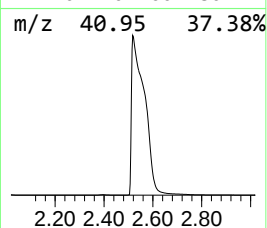
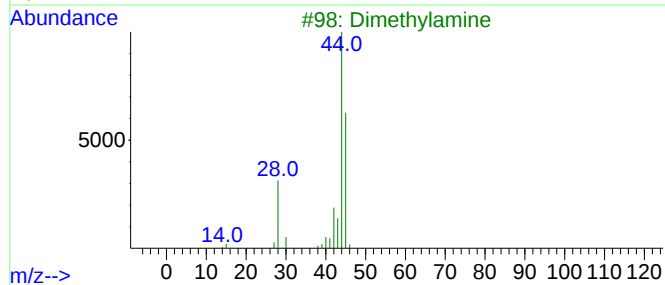
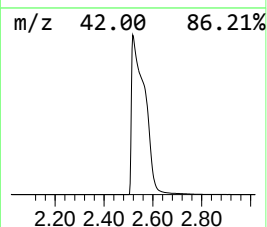
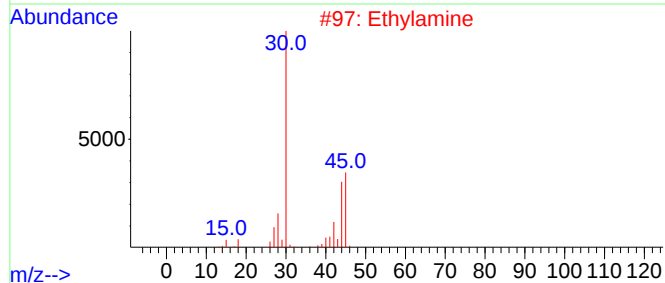
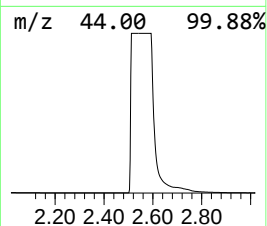
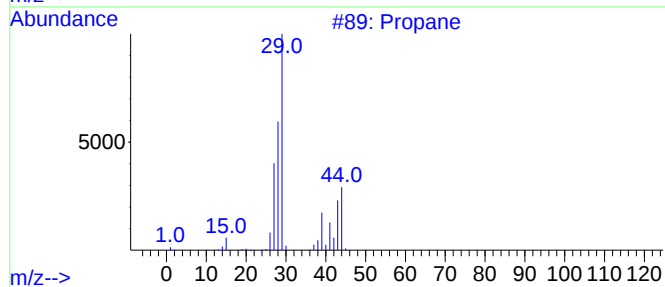
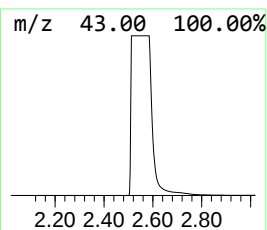
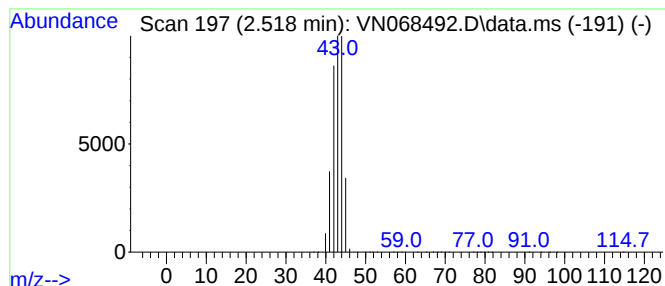
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.518 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.518	3388.92 ug/l	205275000	Pentafluorobenzene	8.086	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane	44	C3H8	000074-98-6	5
2	Ethylamine	45	C2H7N	000075-04-7	4
3	Dimethylamine	45	C2H7N	000124-40-3	3
4	Ethylene oxide	44	C2H4O	000075-21-8	3
5	Acetonitrile-d3	44	C2D3N	002206-26-0	3



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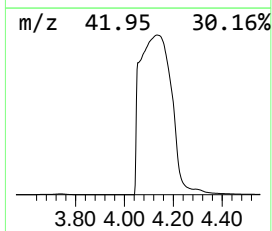
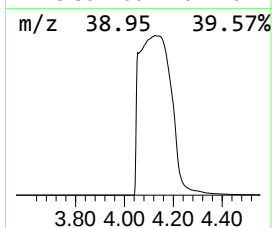
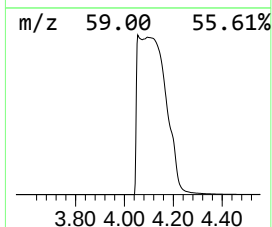
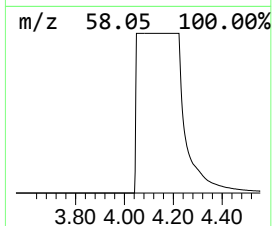
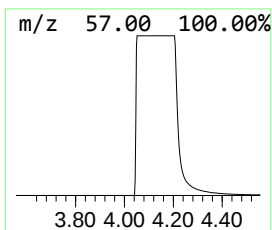
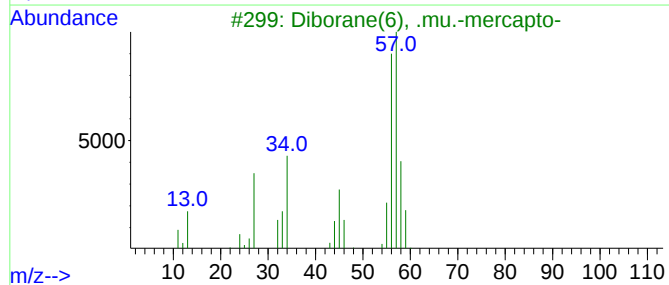
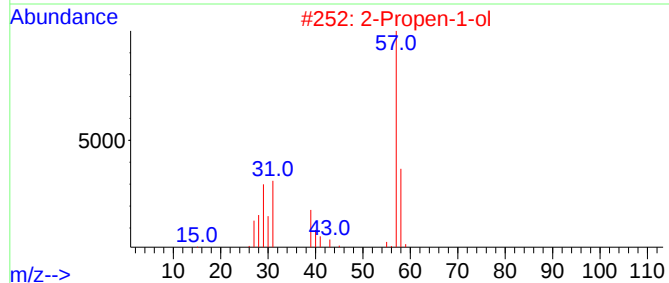
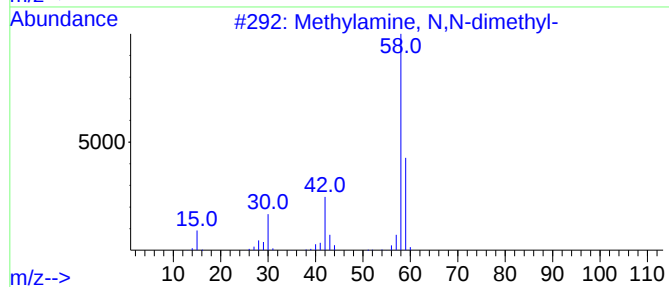
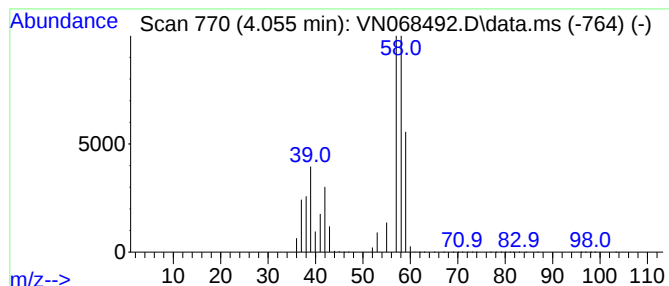
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 unknown4.055 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.055	523.64 ug/l	31718300	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methylamine, N,N-dimethyl-	59	C3H9N	000075-50-3	27
2			2-Propen-1-ol	58	C3H6O	000107-18-6	7
3			Diborane(6), .mu.-mercapto-	60	B2H6S	022548-43-2	5
4			Ethene, methoxy-	58	C3H6O	000107-25-5	4
5			tert-Butyl N-hydroxycarbamate	133	C5H11NO3	036016-38-3	4



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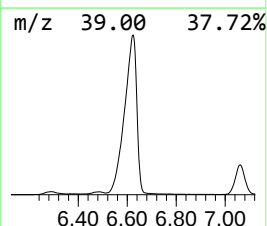
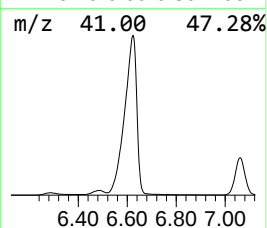
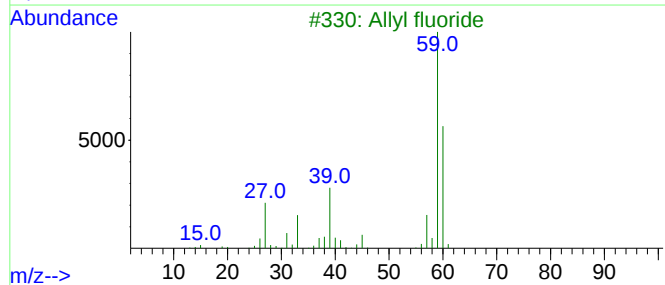
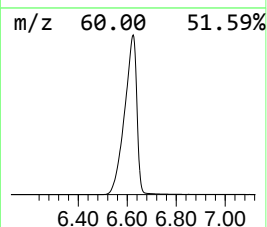
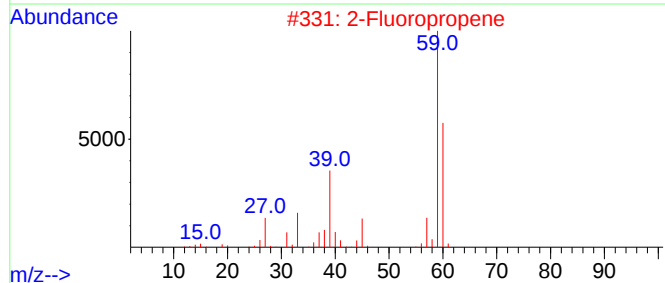
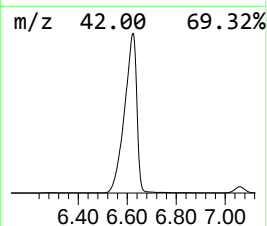
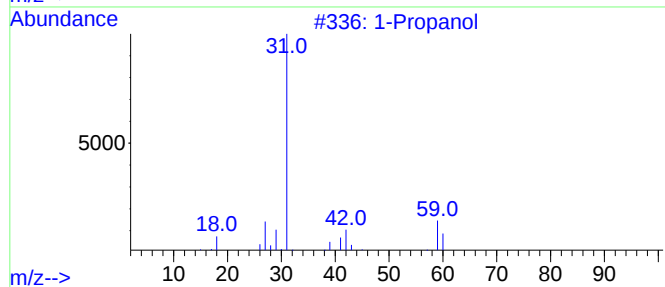
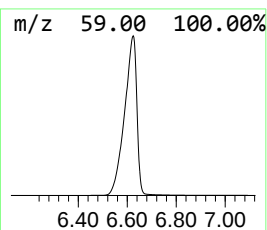
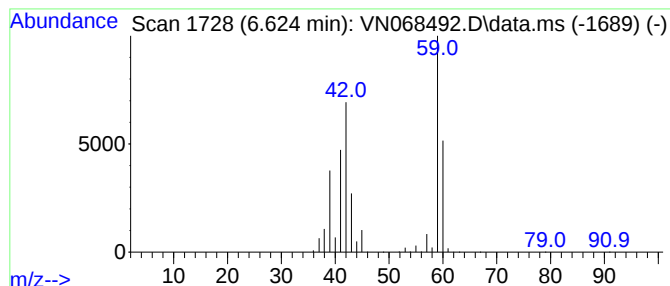
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Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.624	533.58 ug/l	32320000	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol			60	C3H8O	000071-23-8	78
2	2-Fluoropropene			60	C3H5F	001184-60-7	50
3	Allyl fluoride			60	C3H5F	000818-92-8	42
4	Formamidoxime			60	CH4N2O	000624-82-8	27
5	Cyclopropane			42	C3H6	000075-19-4	10



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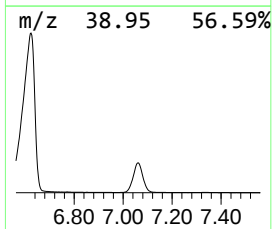
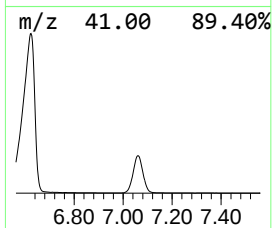
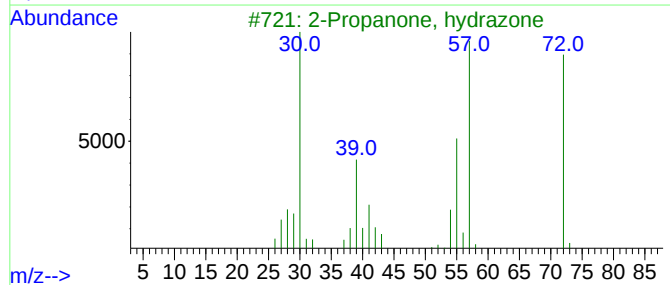
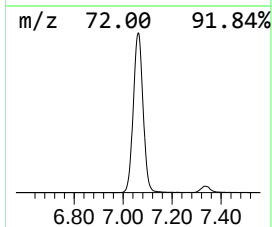
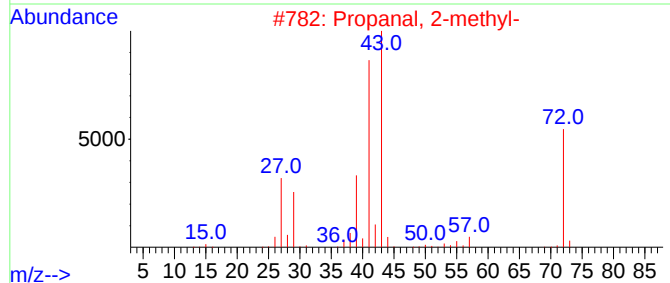
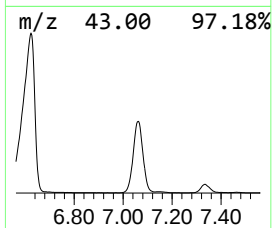
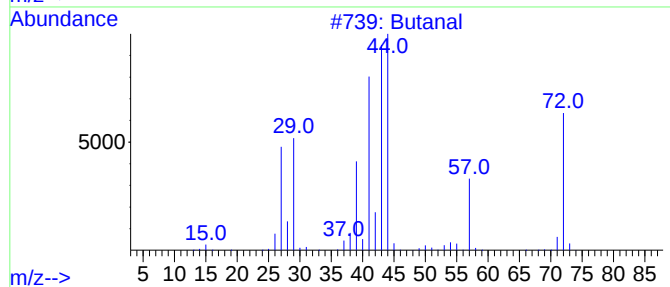
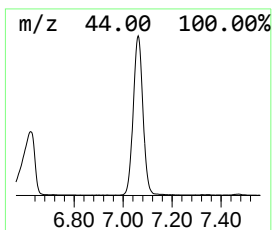
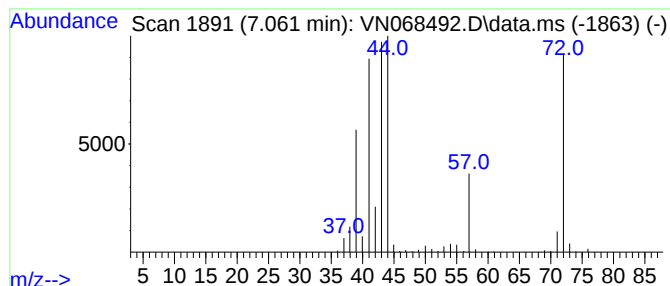
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Peak Number 4 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.061	76.34 ug/l	4624030	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	38
3			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	35
4			Propane	44	C3H8	000074-98-6	35
5			O-Methylisourea	74	C2H6N2O	002440-60-0	25



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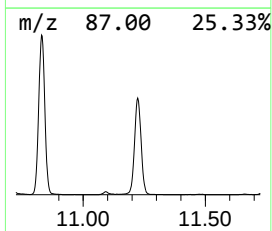
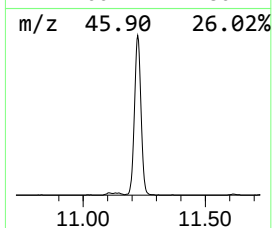
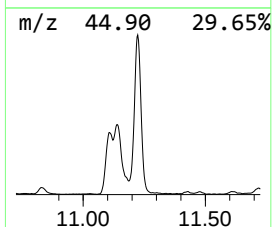
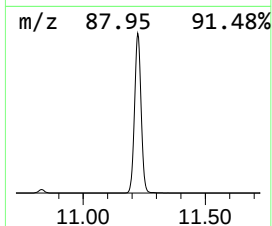
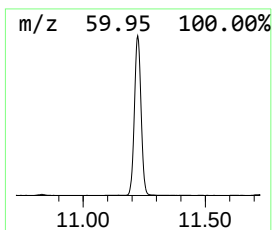
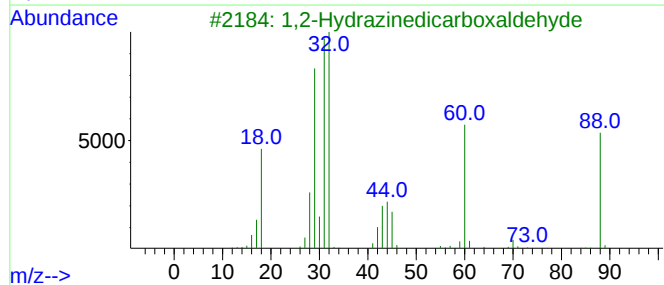
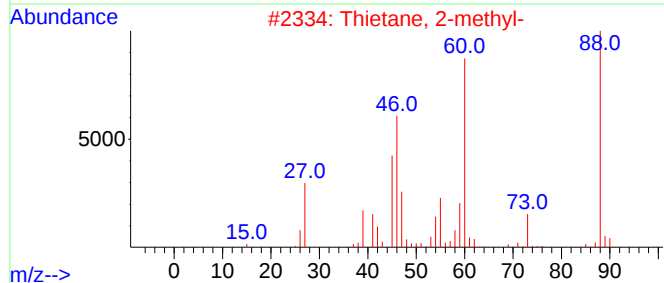
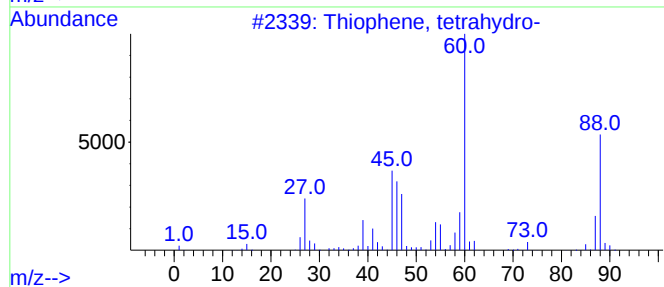
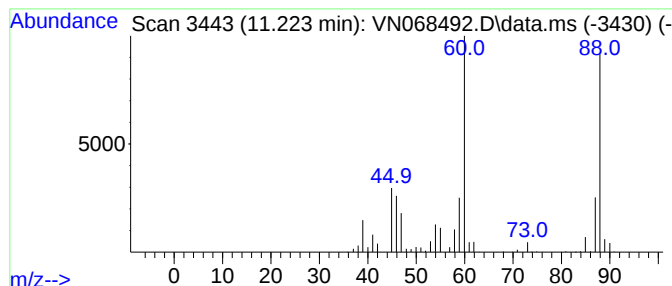
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Peak Number 5 Thiophene, tetrahydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.224	17.67 ug/l	2739470	Chlorobenzene-d5	11.746

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	93
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	36
4			Sulfide, allyl methyl	88	C4H8S	010152-76-8	32
5			2,2-Dimethylthiirane	88	C4H8S	003772-13-2	25



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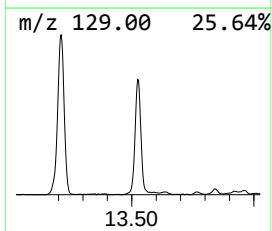
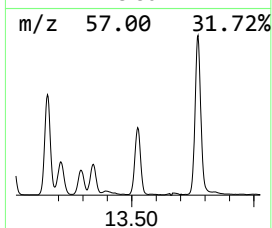
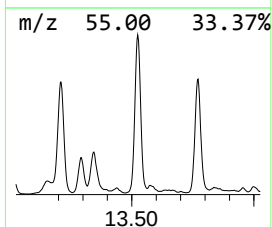
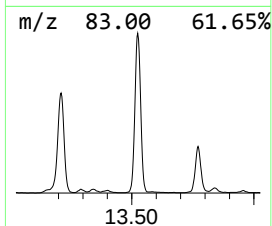
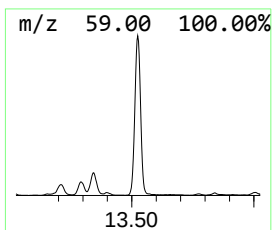
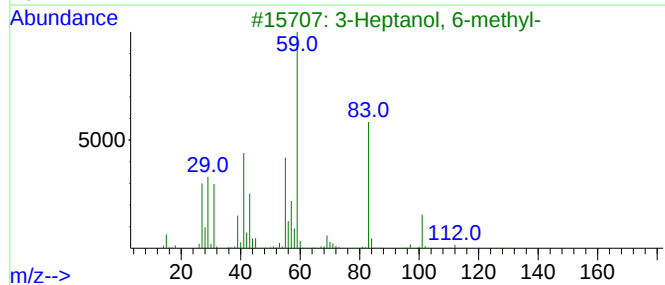
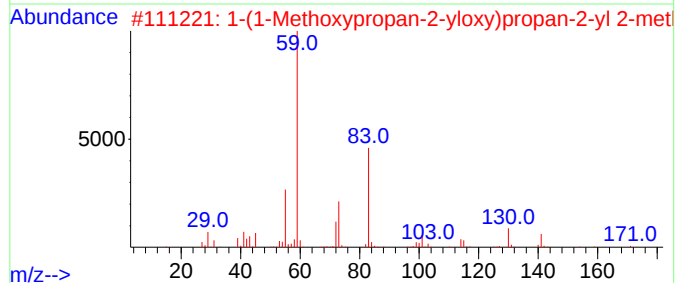
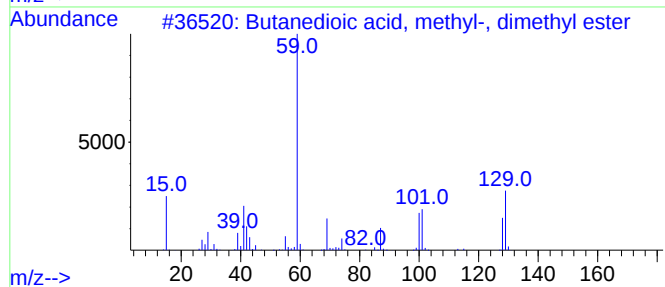
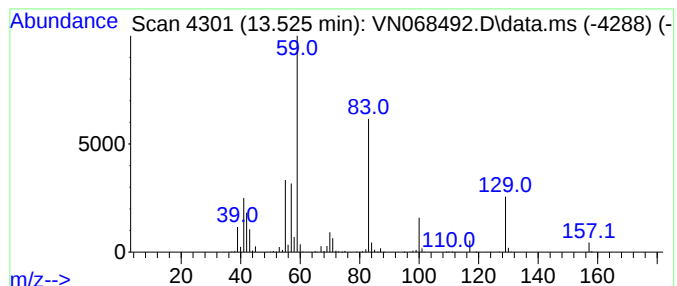
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 6 unknown13.525 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.525	38.89 ug/l	2194550	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanedioic acid, methyl-, dimet...	160	C7H12O4	001604-11-1	47
2			1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	42
3			3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	40
4			3-Hexene, 1-(1-methoxyethoxy)-, ...	158	C9H18O2	054340-97-5	40
5			3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068492.D
Acq On : 15 Sep 2021 18:40
Operator : JC/MD
Sample : M3759-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31207

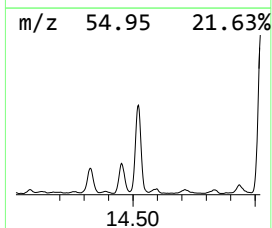
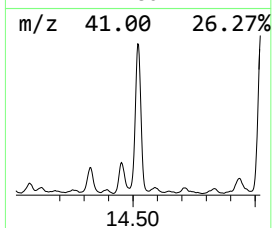
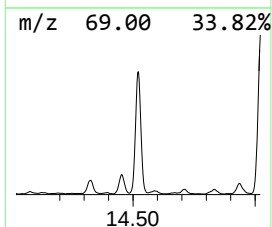
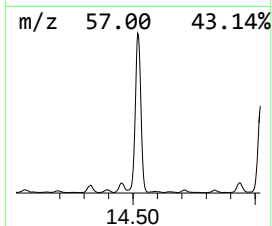
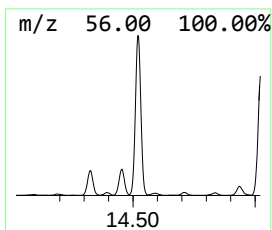
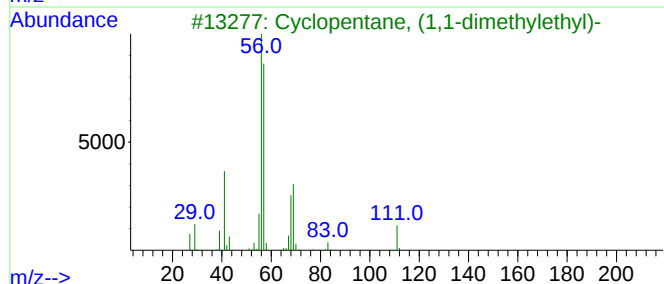
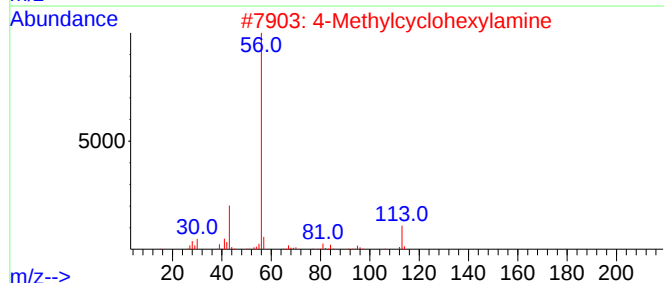
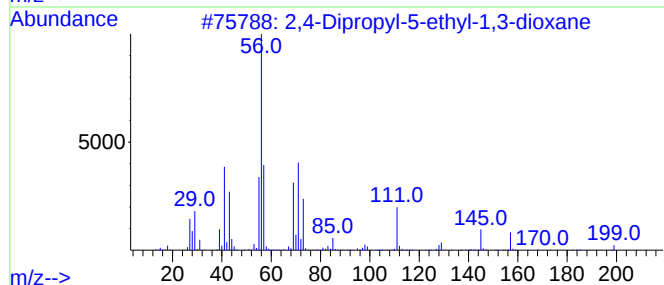
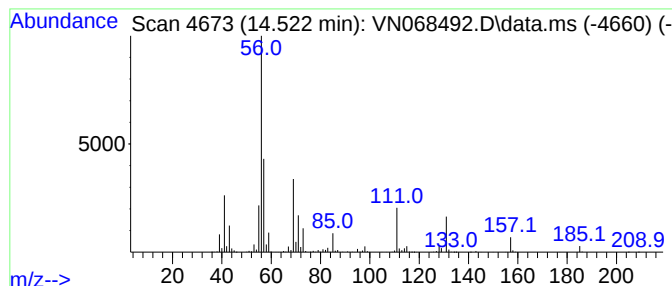
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 7 2,4-Dipropyl-5-ethyl-1,3-di... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.522	51.83 ug/l	2924720	1,4-Dichlorobenzene-d4	13.678

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	59
2		4-Methylcyclohexylamine	113	C7H15N	006321-23-9	43
3		Cyclopentane, (1,1-dimethylethyl)-	126	C9H18	003875-52-3	38
4		Cyclopentanamine	85	C5H11N	001003-03-8	38
5		2H-Azepin-2-one, 3-aminohexahydro-	128	C6H12N2O	000671-42-1	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068492.D
Acq On : 15 Sep 2021 18:40
Operator : JC/MD
Sample : M3759-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31207

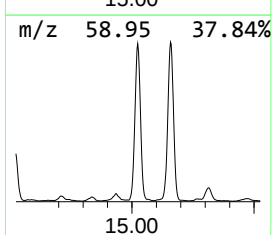
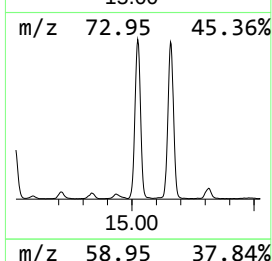
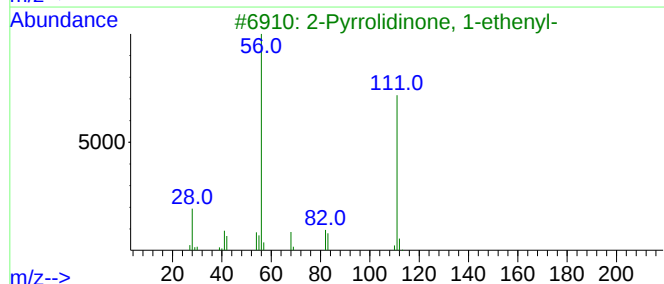
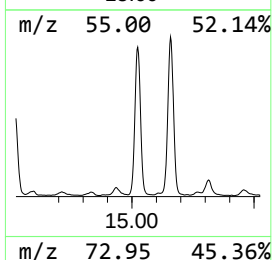
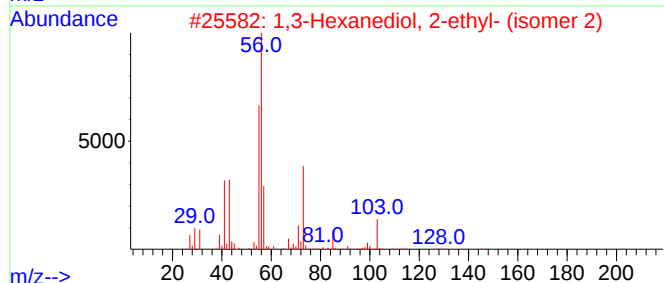
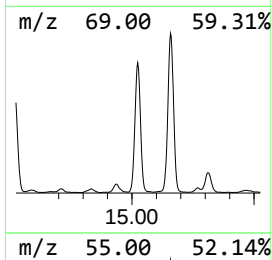
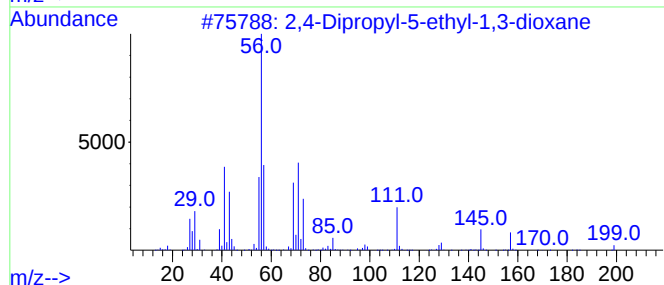
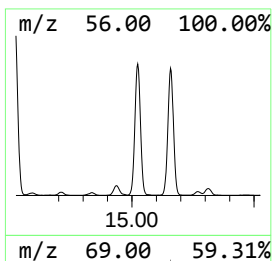
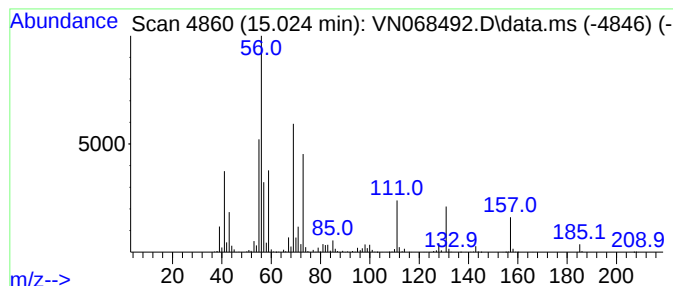
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 8 unknown15.024 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.024	58.64 ug/l	3308500	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	42
2			1,3-Hexanediol, 2-ethyl- (isomer 2)	146	C8H18O2	1000484-18-1	37
3			2-Pyrrolidinone, 1-ethenyl-	111	C6H9NO	000088-12-0	37
4			1,3-Hexanediol, 2-ethyl- (isomer 1)	146	C8H18O2	1000484-18-2	37
5			1-Hexene, 2-methyl-	98	C7H14	006094-02-6	35



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068492.D
Acq On : 15 Sep 2021 18:40
Operator : JC/MD
Sample : M3759-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31207

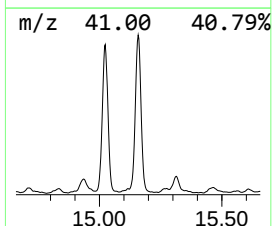
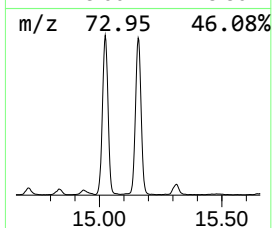
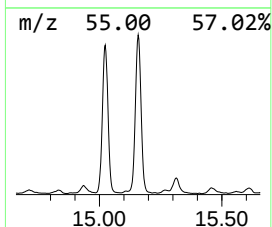
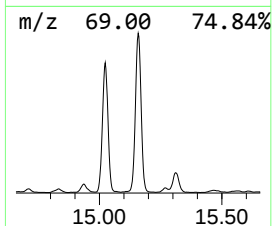
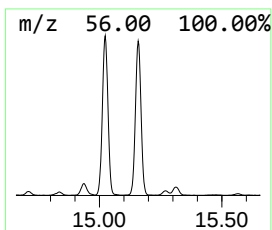
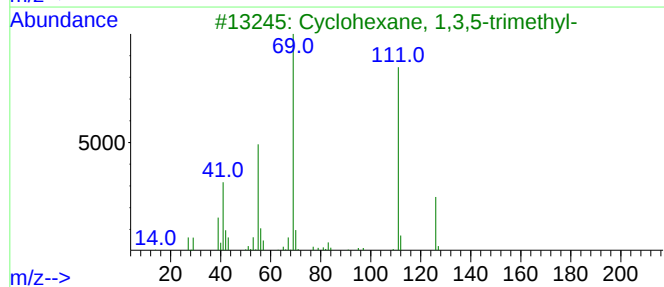
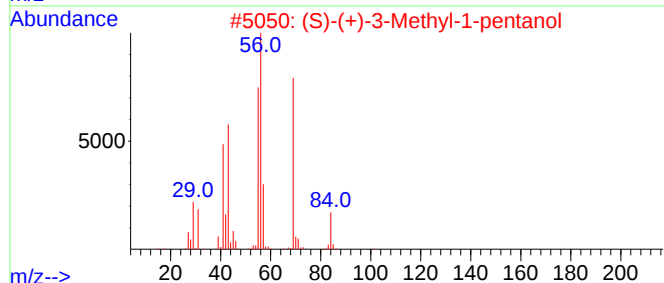
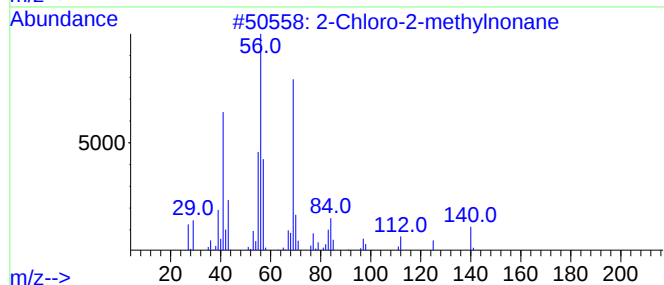
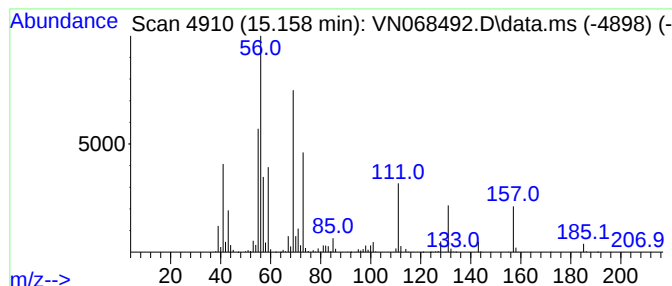
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.158 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.158	65.40 ug/l	3690480	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloro-2-methylnonane	176	C10H21Cl	004325-50-2	37
2			(S)-(+)-3-Methyl-1-pentanol	102	C6H14O	042072-39-9	37
3			Cyclohexane, 1,3,5-trimethyl-	126	C9H18	001839-63-0	22
4			6-Methyl-hept-2-yn-4-ol	126	C8H14O	060018-69-1	22
5			Undecanol-4	172	C11H24O	004272-06-4	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
Data File : VN068492.D
Acq On : 15 Sep 2021 18:40
Operator : JC/MD
Sample : M3759-10
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
31207

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown4.055	4.055	523.6	ug/l	31718300	1	8.086	3028620	50.0
1-Propanol	6.624	533.6	ug/l	32320000	1	8.086	3028620	50.0
Butanal	7.061	76.3	ug/l	4624030	1	8.086	3028620	50.0
Thiophene, tetr...	11.224	17.7	ug/l	2739470	3	11.746	7750190	50.0
unknown13.525	13.525	38.9	ug/l	2194550	4	13.678	2821260	50.0
2,4-Dipropyl-5-...	14.522	51.8	ug/l	2924720	4	13.678	2821260	50.0
unknown15.024	15.024	58.6	ug/l	3308500	4	13.678	2821260	50.0
unknown15.158	15.158	65.4	ug/l	3690480	4	13.678	2821260	50.0