

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091521\
 Data File : VN068493.D
 Acq On : 15 Sep 2021 19:06
 Operator : JC/MD
 Sample : M3759-11
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31208

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: VN068493.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.558	197	212	264	rBV3	39688487	97708299	100.00%	42.934%
2	4.073	771	777	781	rBV3	51467974	57936945	59.30%	25.458%
3	6.605	1688	1721	1776	rVB	6003795	18804780	19.25%	8.263%
4	7.058	1866	1890	1918	rBV3	495463	1412488	1.45%	0.621%
5	8.021	2224	2249	2260	rBV2	595764	1439179	1.47%	0.632%
6	8.086	2260	2273	2302	rVB	1273179	2841625	2.91%	1.249%
7	8.437	2379	2404	2428	rBV3	559908	1401828	1.43%	0.616%
8	8.968	2585	2602	2626	rVB	1460156	2978855	3.05%	1.309%
9	10.443	3133	3152	3162	rBV	2302276	4289089	4.39%	1.885%
10	10.507	3162	3176	3199	rVV	10629109	19592710	20.05%	8.609%
11	11.714	3612	3626	3632	rBV	2375134	4347226	4.45%	1.910%
12	11.848	3663	3676	3699	rBV	625655	1452766	1.49%	0.638%
13	11.950	3700	3714	3743	rVB	2350032	4591876	4.70%	2.018%
14	12.283	3809	3838	3869	rBV	1066976	2121544	2.17%	0.932%
15	12.734	3995	4006	4035	rVB2	1437523	2616684	2.68%	1.150%
16	13.214	4173	4185	4203	rVB3	536444	1097376	1.12%	0.482%
17	13.678	4343	4358	4381	rBV2	1558828	2942208	3.01%	1.293%

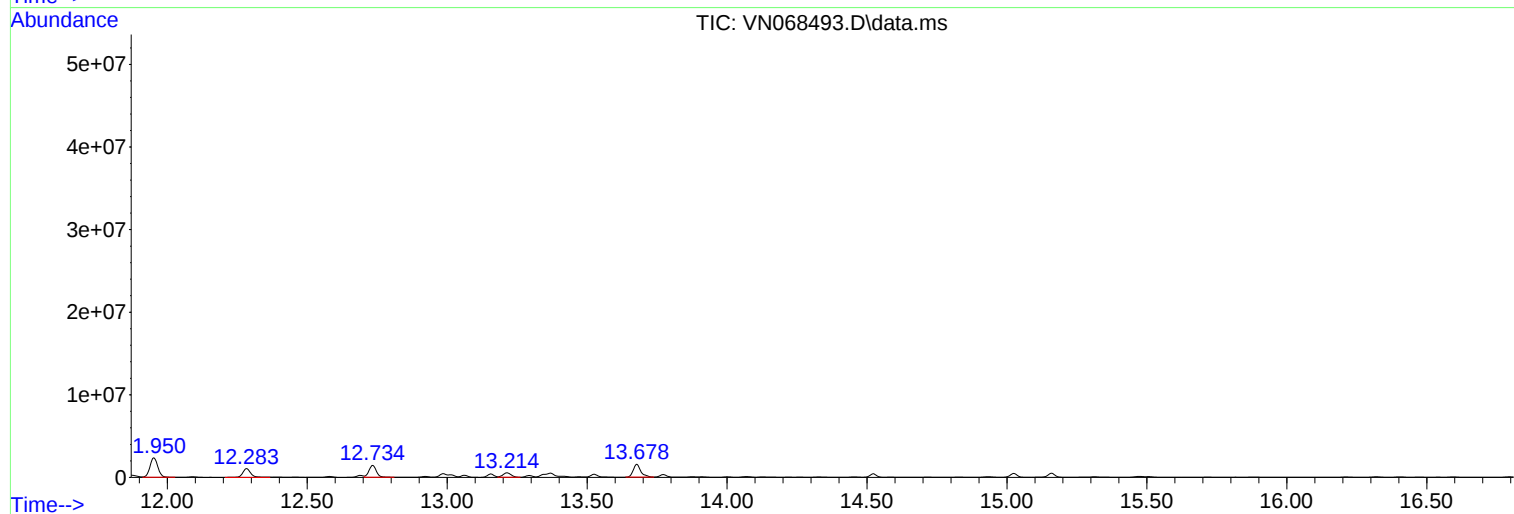
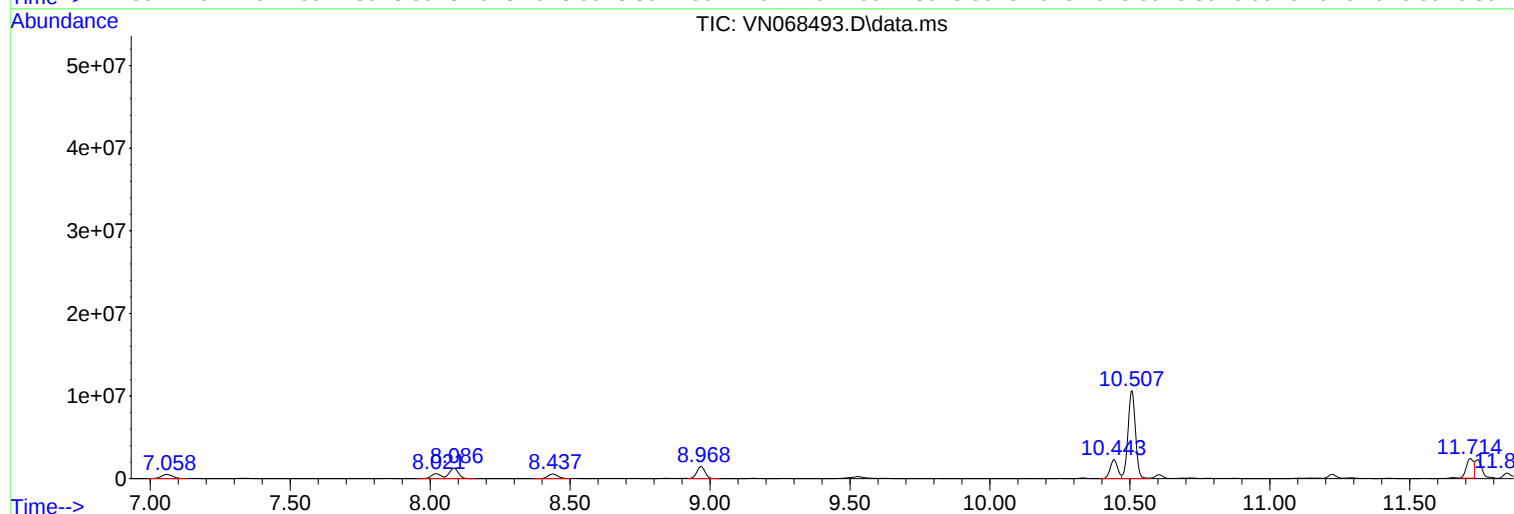
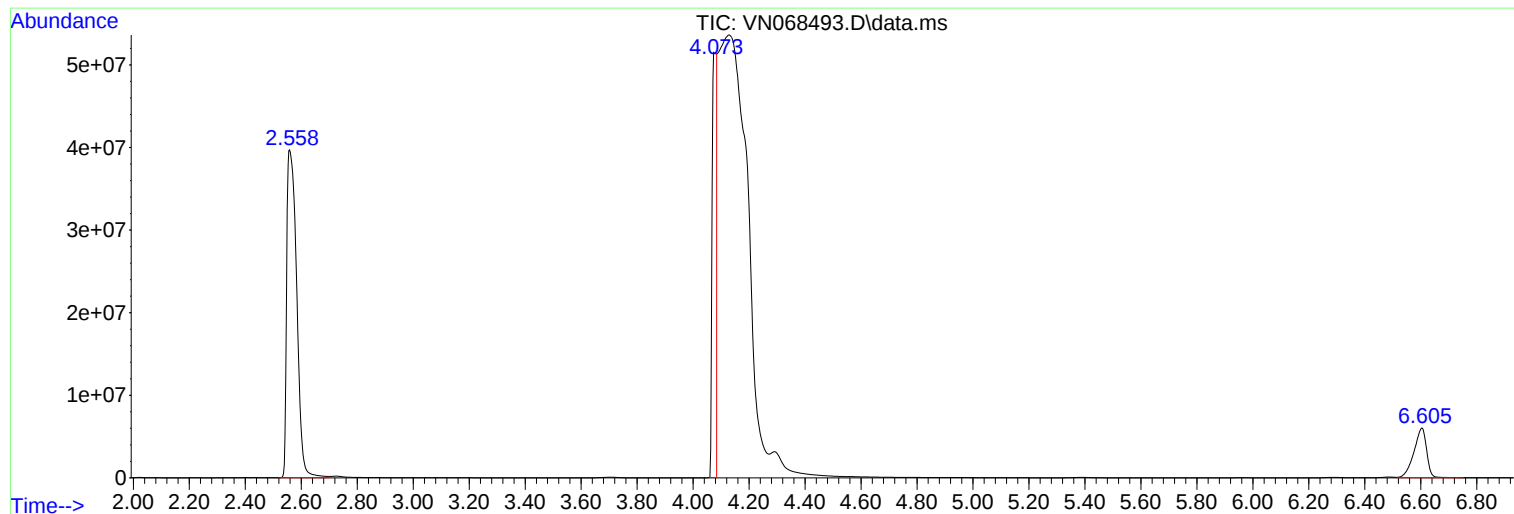
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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



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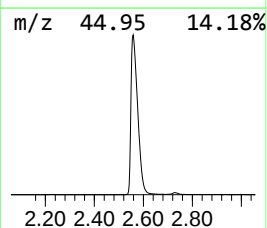
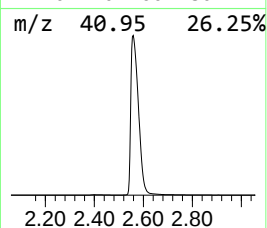
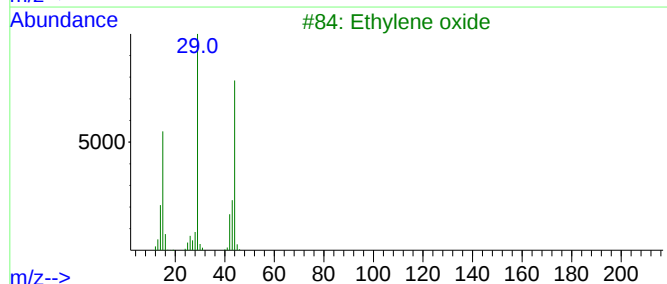
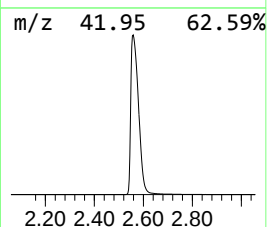
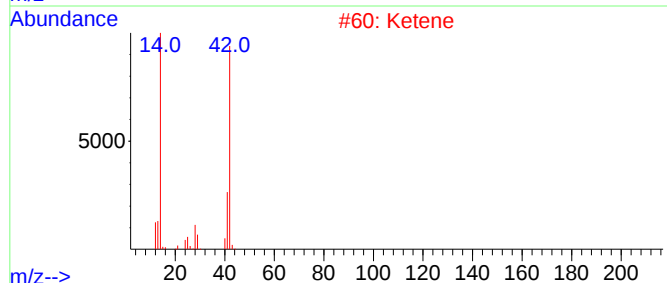
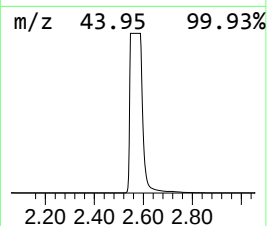
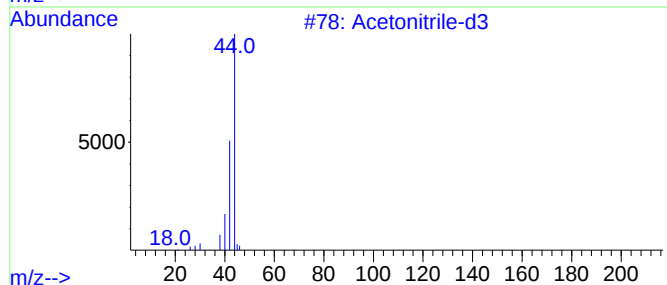
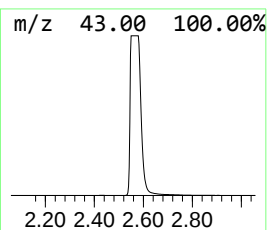
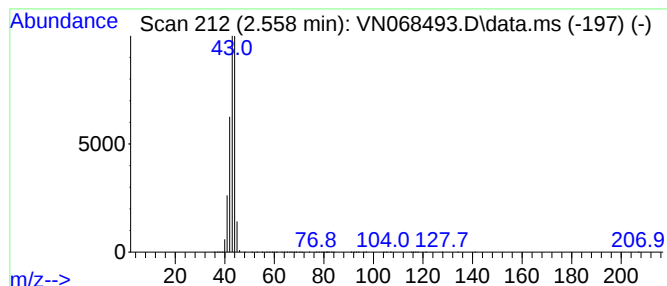
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.558 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.558	1719.23 ug/l	97708300	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetonitrile-d3	44	C2D3N	002206-26-0	4
2		Ketene	42	C2H2O	000463-51-4	4
3		Ethylene oxide	44	C2H4O	000075-21-8	3
4		Propane	44	C3H8	000074-98-6	3
5		Methane, diazo-	42	CH2N2	000334-88-3	3



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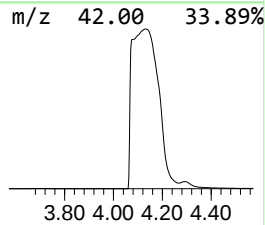
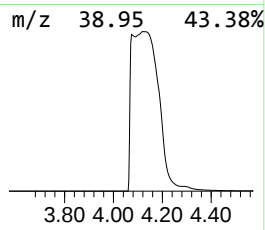
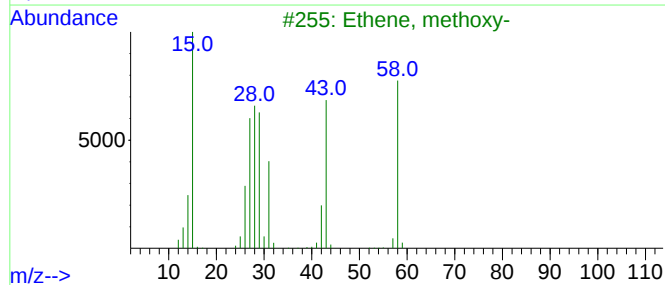
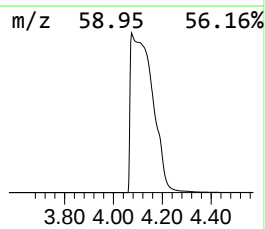
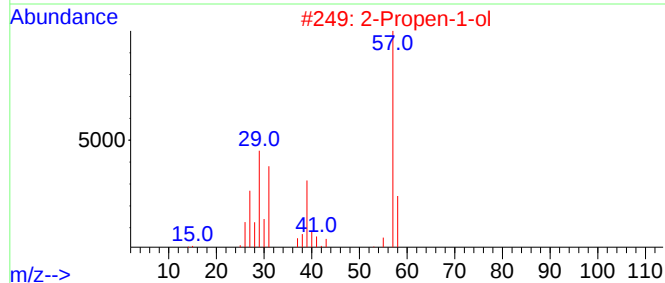
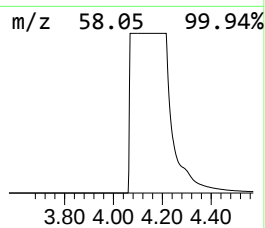
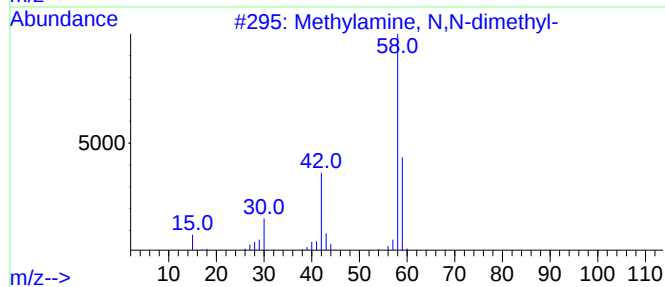
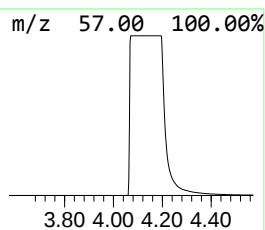
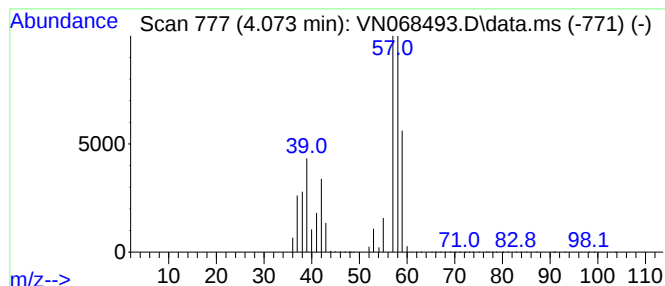
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown4.073 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.073	1019.43 ug/l	57936900	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		Ethene, methoxy-	58	C3H6O	000107-25-5	4
4		Succindialdehyde	86	C4H6O2	000638-37-9	4
5		Propanal	58	C3H6O	000123-38-6	4



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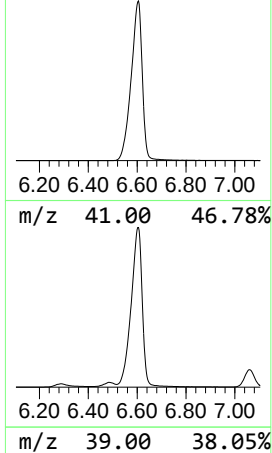
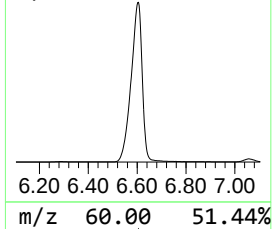
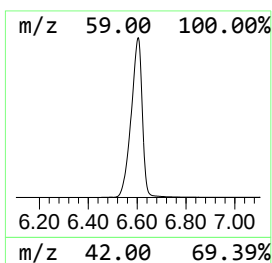
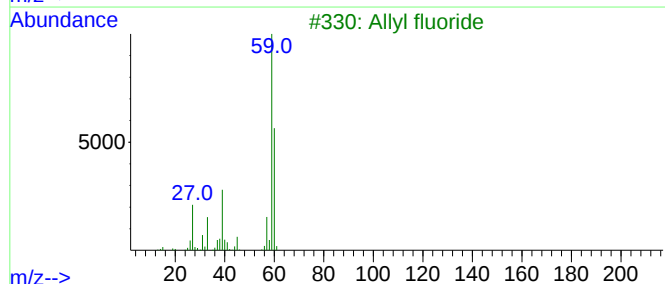
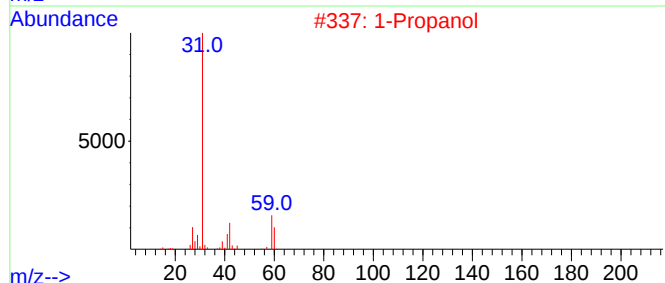
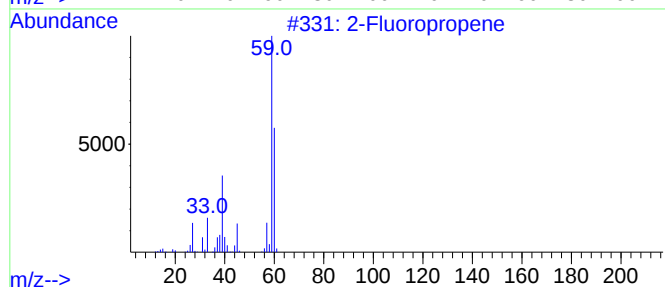
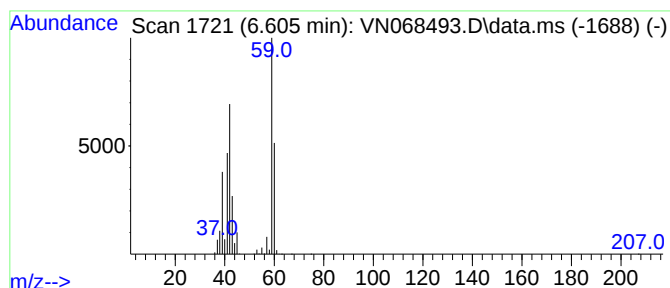
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Quant Title : SW846 8260

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

Peak Number 3 2-Fluoropropene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.605	330.88 ug/l	18804800	Pentafluorobenzene	8.086

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Fluoropropene	60	C3H5F	001184-60-7	59
2		1-Propanol	60	C3H8O	000071-23-8	59
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Formamidoxime	60	CH4N2O	000624-82-8	22
5		Cyclopropane	42	C3H6	000075-19-4	16



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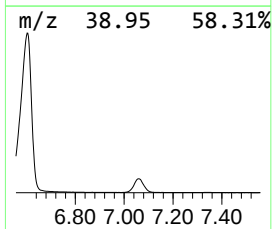
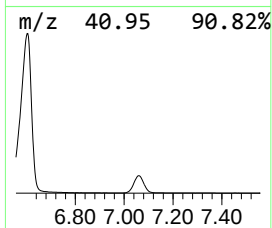
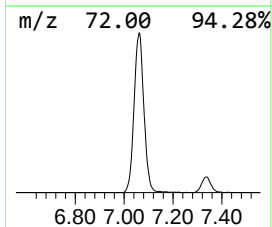
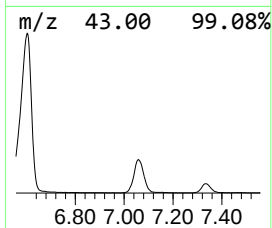
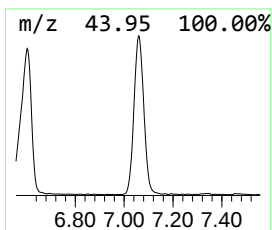
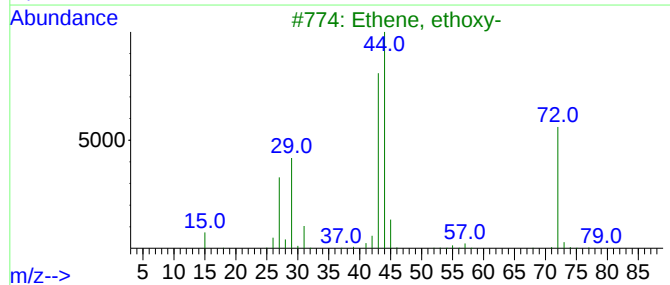
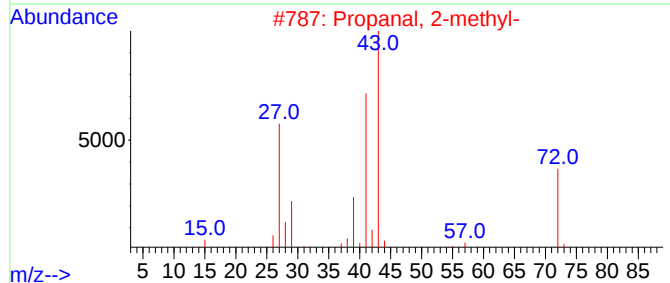
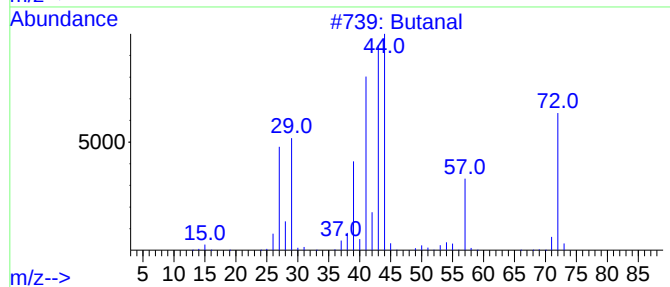
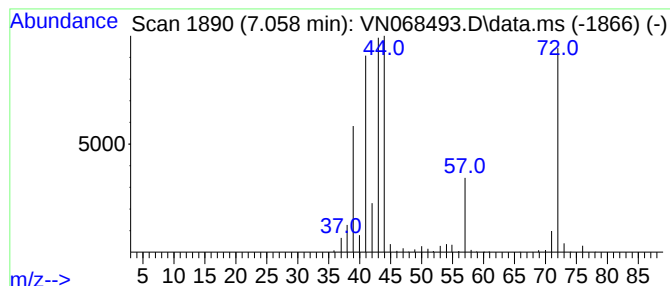
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N090721W.M
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Peak Number 4 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.058	24.85 ug/l	1412490	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	43
3			Ethene, ethoxy-	72	C4H8O	000109-92-2	42
4			2-Propanone, hydrazone	72	C3H8N2	005281-20-9	38
5			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	28



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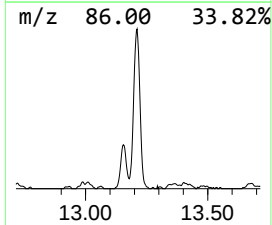
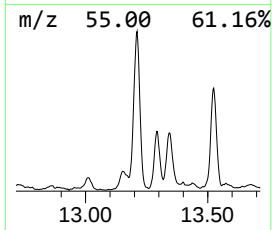
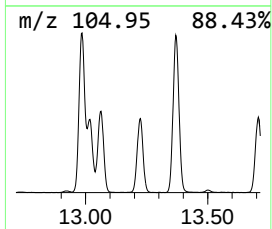
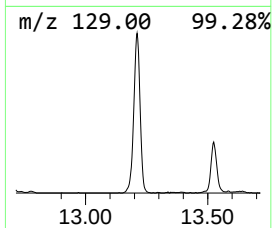
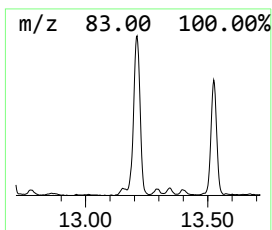
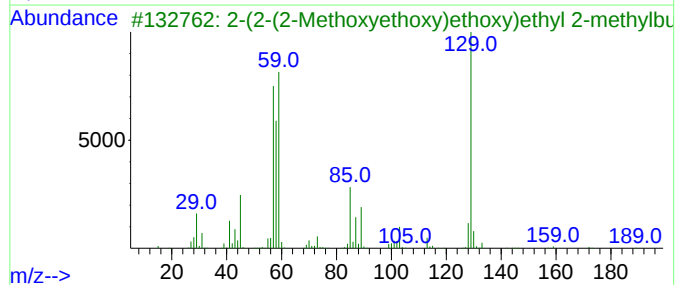
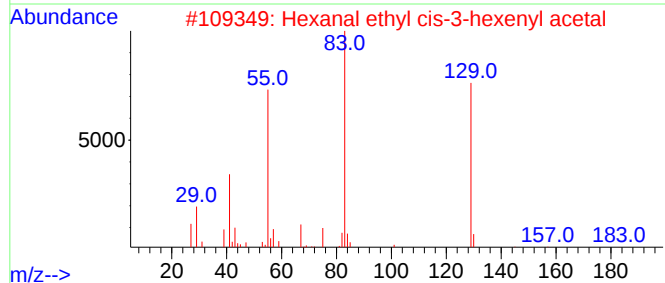
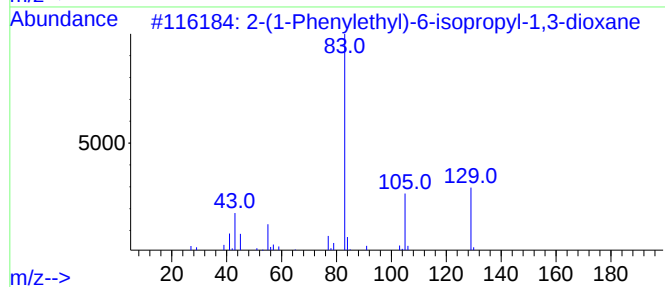
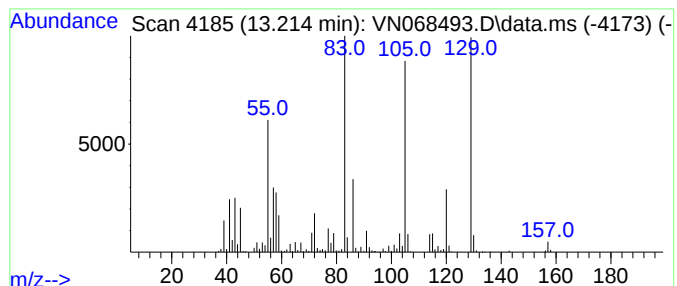
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-(1-Phenylethyl)-6-isoprop... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.214	18.65 ug/l	1097380	1,4-Dichlorobenzene-d4	13.678

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-(1-Phenylethyl)-6-isopropyl-1,...	234	C15H22O2	1000431-40-0	53
2			Hexanal ethyl cis-3-hexenyl acetal	228	C14H28O2	1000431-42-9	37
3			2-(2-(2-Methoxyethoxy)ethoxy)eth...	248	C12H24O5	1000366-97-4	16
4			1H-Imidazol-2-amine	83	C3H5N3	007720-39-0	10
5			3,3-Diethoxy-1-propyne	128	C7H12O2	010160-87-9	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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unknown4.073	4.073	1019.4	ug/l	57936900	1	8.086	2841630	50.0
2-Fluoropropene	6.605	330.9	ug/l	18804800	1	8.086	2841630	50.0
Butanal	7.058	24.9	ug/l	1412490	1	8.086	2841630	50.0
2-(1-Phenylethy...	13.214	18.6	ug/l	1097380	4	13.678	2942210	50.0