

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
 Data File : VN067126.D
 Acq On : 18 May 2021 14:52
 Operator : JC/MD
 Sample : M2387-06 20X
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 41799

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\82N051421W.M

Title : SW846 8260

Signal : TIC: VN067126.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.303	196	210	239	rBV	764017	1288274	6.81%	2.917%
2	6.567	1780	1800	1832	rBV	91438	281897	1.49%	0.638%
3	7.519	2132	2155	2169	rBV2	376392	966107	5.11%	2.187%
4	7.597	2170	2184	2217	rVB	680467	1659426	8.77%	3.757%
5	7.959	2297	2319	2351	rBV2	383073	925410	4.89%	2.095%
6	8.530	2506	2532	2581	rBV2	8837809	18915548	100.00%	42.823%
7	8.780	2605	2625	2643	rBV	3891380	7806195	41.27%	17.673%
8	10.037	3074	3094	3132	rBV	1528875	2898952	15.33%	6.563%
9	11.357	3570	3586	3623	rBV	1141811	2151983	11.38%	4.872%
10	11.928	3784	3799	3828	rBV2	148652	299259	1.58%	0.677%
11	12.357	3945	3959	4010	rBV	859449	1770496	9.36%	4.008%
12	13.098	4225	4235	4271	rVB4	85098	247603	1.31%	0.561%
13	13.299	4296	4310	4336	rBV	1007304	1943877	10.28%	4.401%
14	13.406	4338	4350	4369	rBV	1749746	3016267	15.95%	6.829%

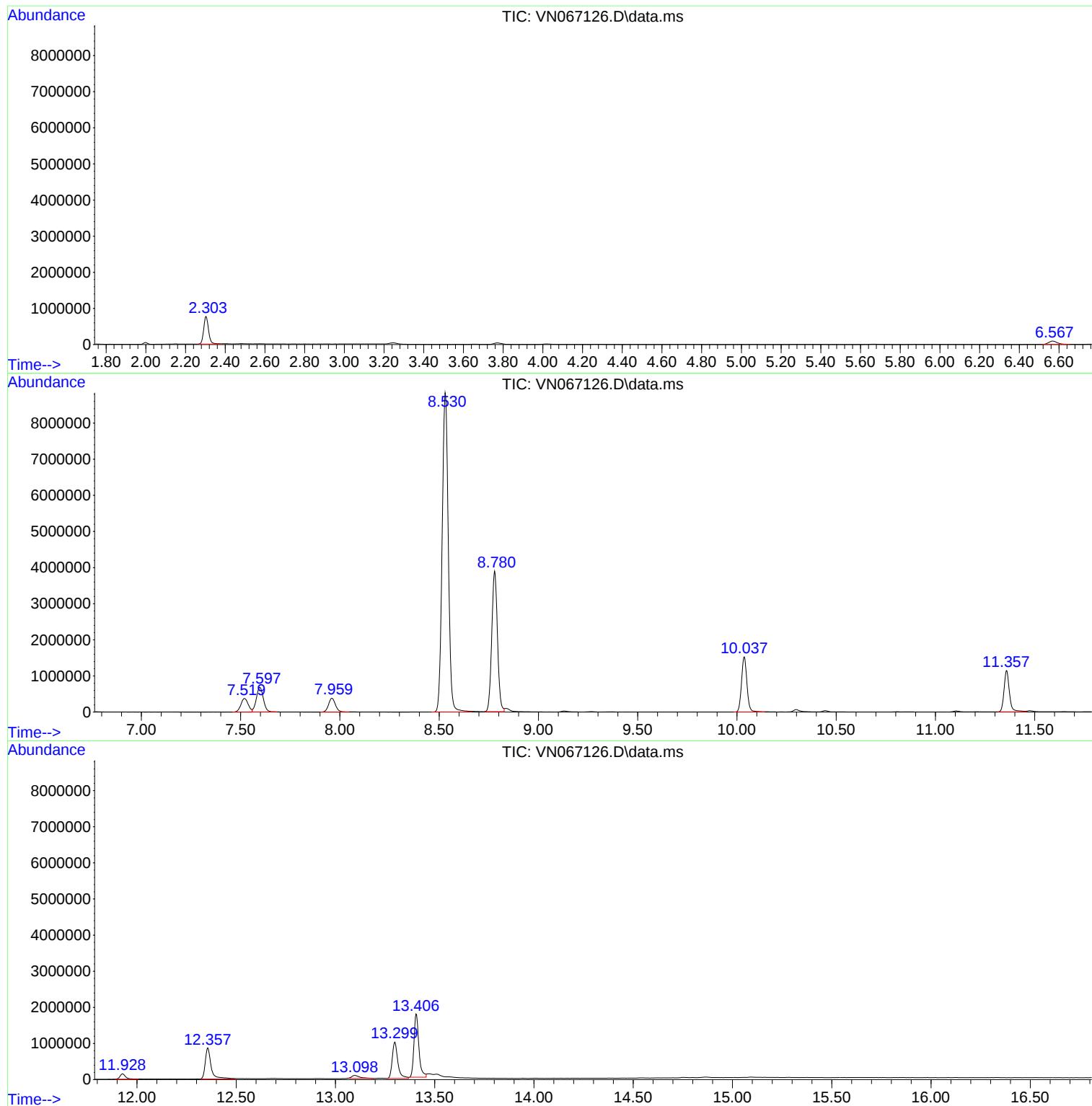
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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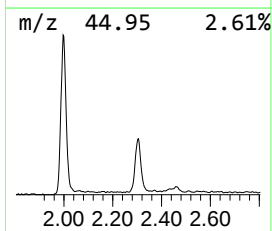
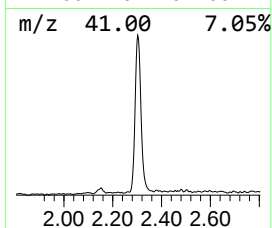
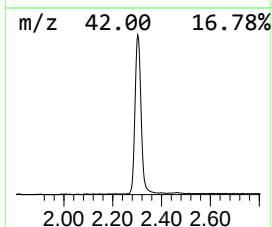
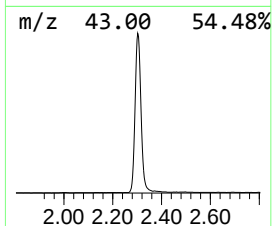
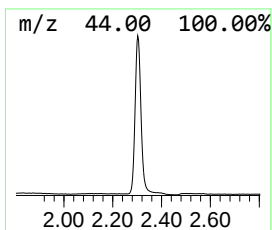
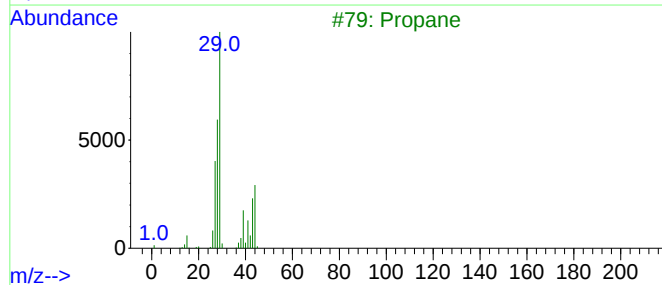
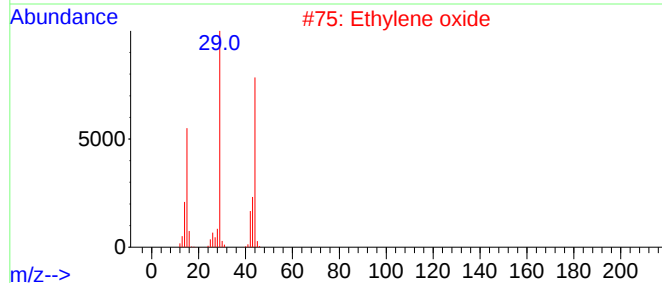
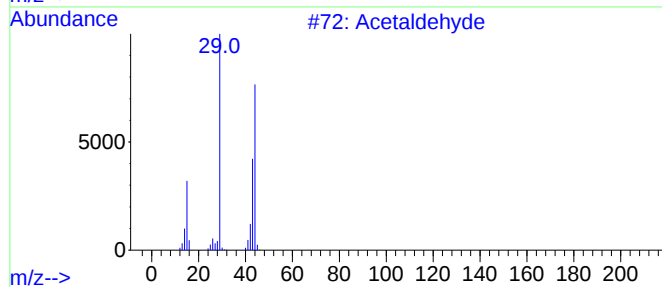
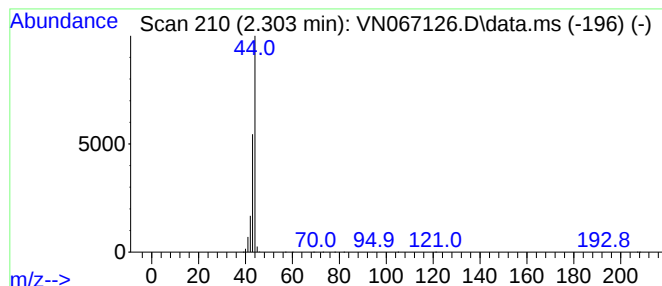
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Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.303	38.82 ug/l	1288270	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	56
2			Ethylene oxide	44	C2H4O	000075-21-8	5
3			Propane	44	C3H8	000074-98-6	4
4			Alanine	89	C3H7NO2	000056-41-7	4
5			1,2-Propanediamine	74	C3H10N2	000078-90-0	4



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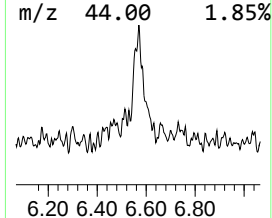
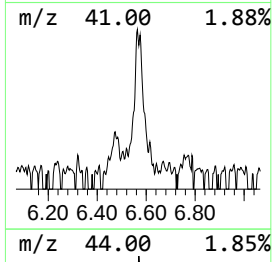
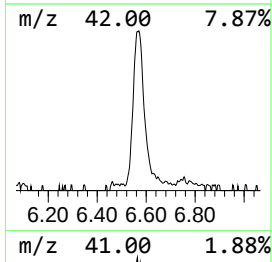
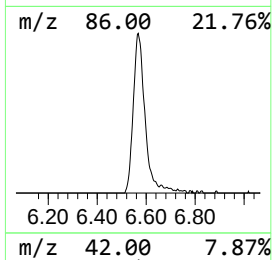
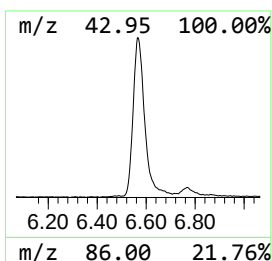
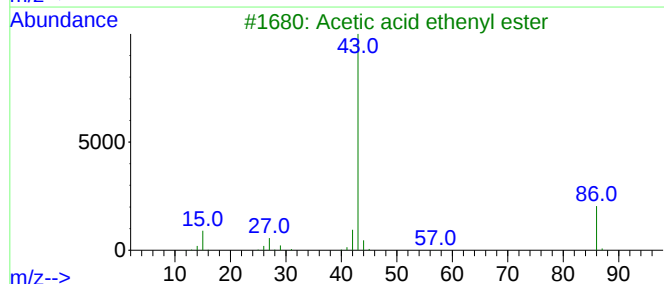
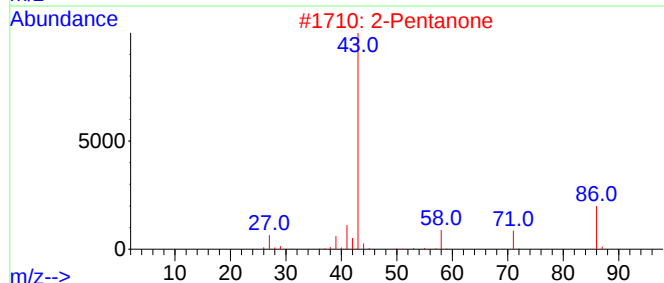
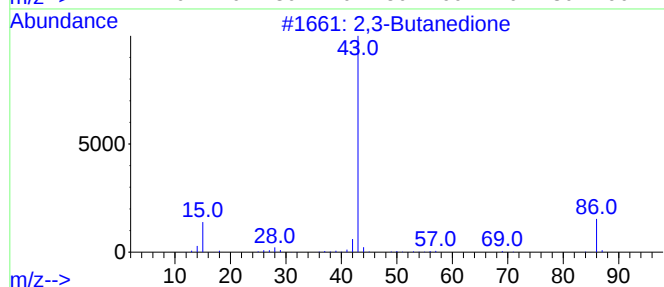
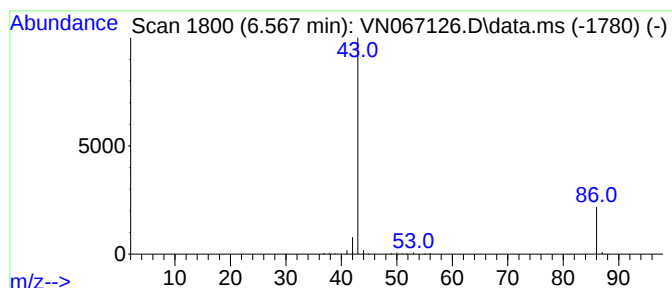
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Peak Number 2 2,3-Butanedione Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.567	8.49 ug/l	281897	Pentafluorobenzene	7.597

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,3-Butanedione			86	C4H6O2	000431-03-8	72
2	2-Pentanone			86	C5H10O	000107-87-9	9
3	Acetic acid ethenyl ester			86	C4H6O2	000108-05-4	9
4	2-Butanone, 3-methyl-			86	C5H10O	000563-80-4	7
5	Ethanone, 1-oxiranyl-			86	C4H6O2	004401-11-0	4



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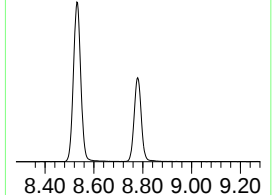
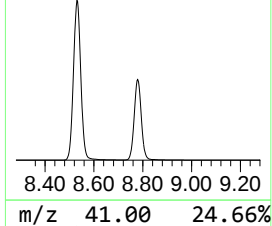
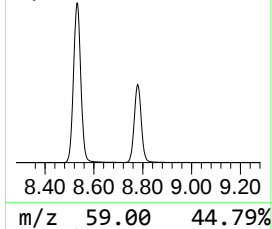
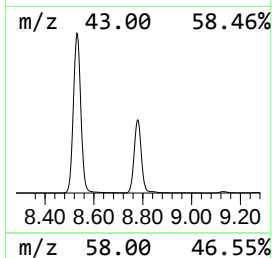
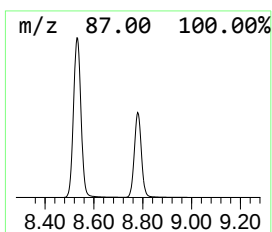
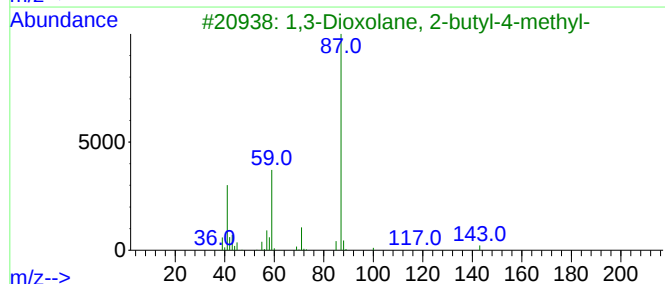
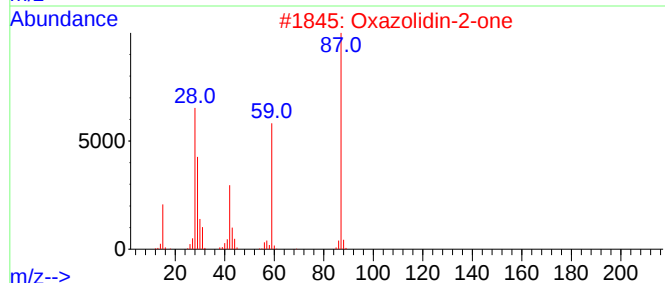
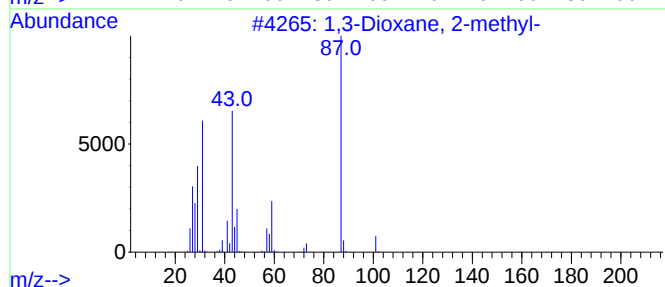
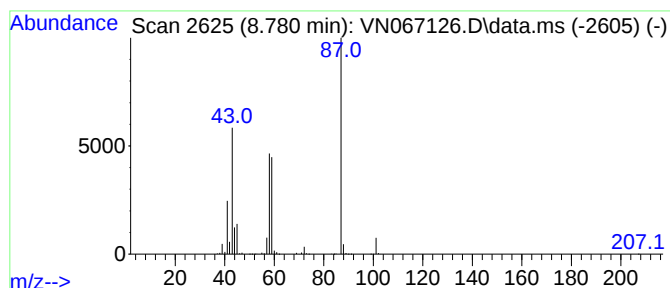
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Peak Number 3 1,3-Dioxane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.780	20.63 ug/l	7806200	1,4-Difluorobenzene	8.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Dioxane, 2-methyl-	102	C5H10O2	000626-68-6	52
2			Oxazolidin-2-one	87	C3H5NO2	000497-25-6	40
3			1,3-Dioxolane, 2-butyl-4-methyl-	144	C8H16O2	074094-60-3	36
4			Ethane, isothiocyanato-	87	C3H5NS	000542-85-8	23
5			N,N-Dimethylacetamide	87	C4H9NO	000127-19-5	9



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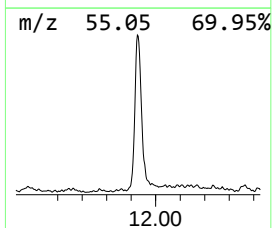
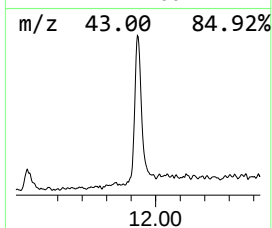
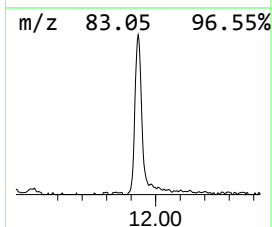
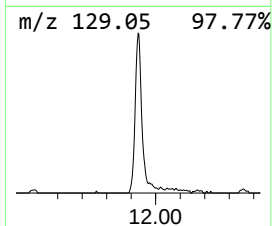
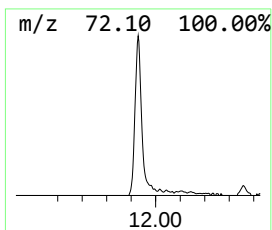
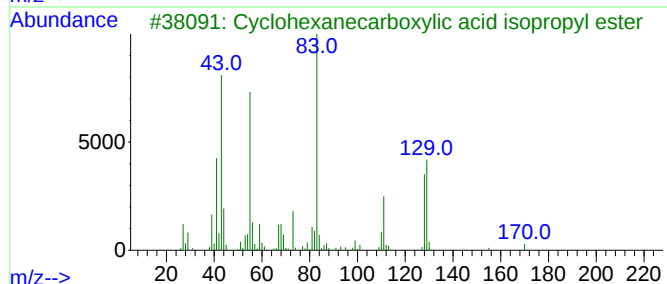
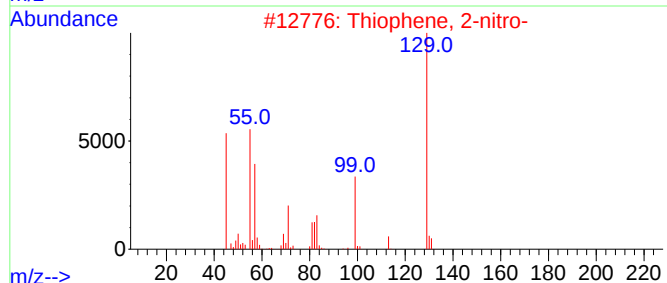
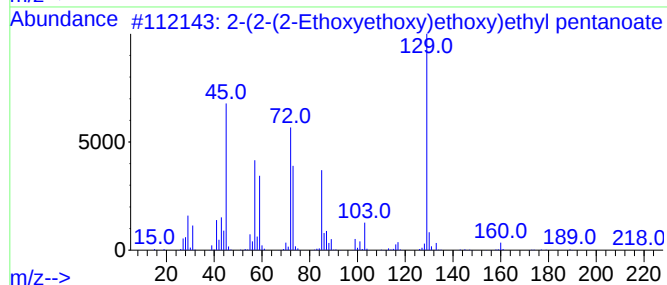
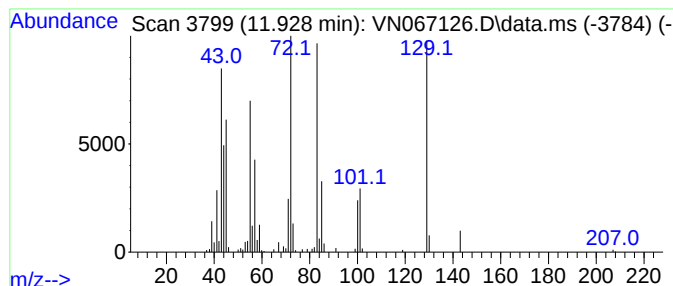
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Peak Number 4 unknown11.928 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.928	6.95 ug/l	299259	Chlorobenzene-d5	11.357

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-(2-(2-Ethoxyethoxy)ethoxy)ethy...	262	C13H26O5	1000367-00-9	35		
2	Thiophene, 2-nitro-	129	C4H3NO2S	000609-40-5	22		
3	Cyclohexanecarboxylic acid isopr...	170	C10H18O2	006553-80-6	22		
4	Cyclohexanecarboxylic acid, 2-me...	184	C11H20O2	037139-85-8	16		
5	Diisopropyl adipate	230	C12H22O4	006938-94-9	14		



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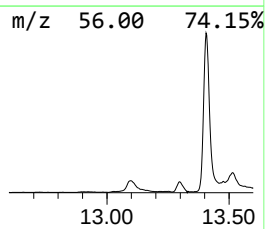
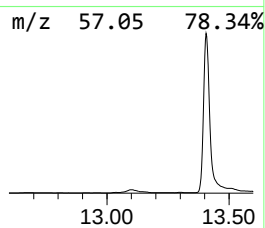
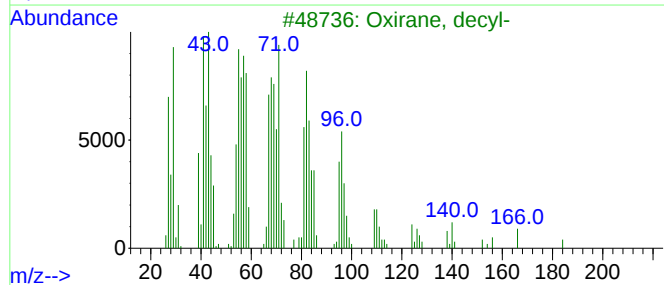
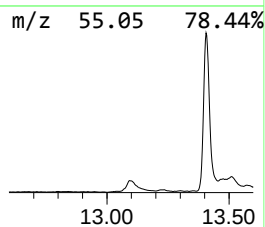
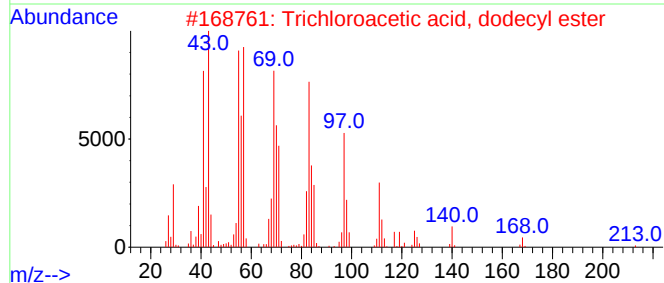
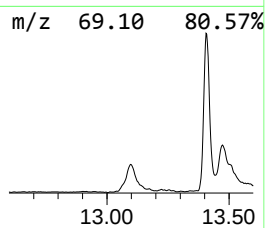
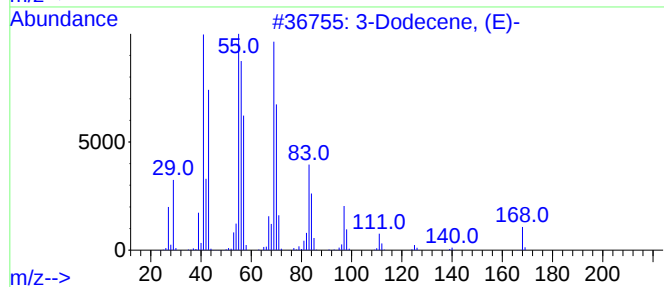
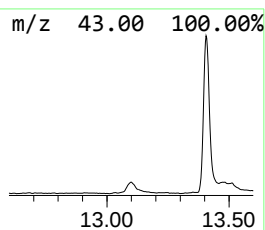
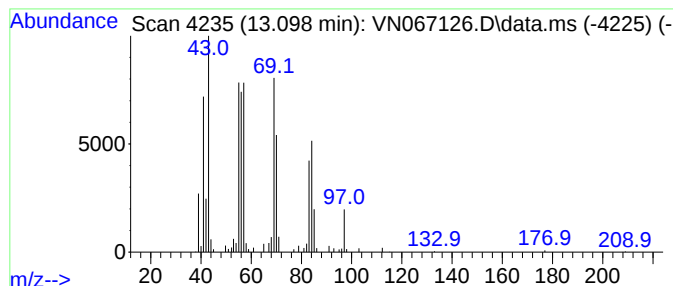
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Peak Number 5 3-Dodecene, (E)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.098	6.37 ug/l	247603	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Dodecene, (E)-	168	C12H24	007206-14-6	72
2			Trichloroacetic acid, dodecyl ester	330	C14H25Cl3O2	074339-50-7	72
3			Oxirane, decyl-	184	C12H24O	002855-19-8	53
4			2-Propyl-1-pentanol, pentafluoro...	276	C11H17F5O2	1000365-51-2	53
5			1-Heptene, 6-methyl-	112	C8H16	005026-76-6	47



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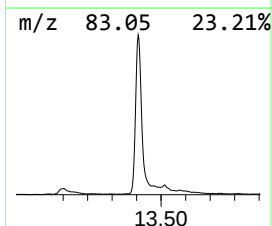
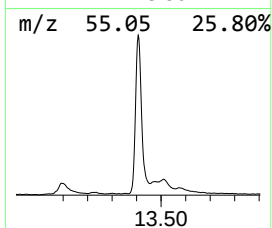
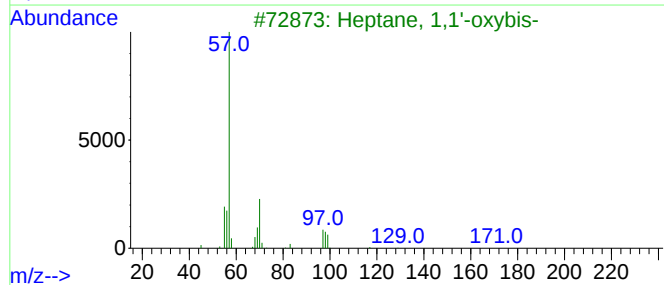
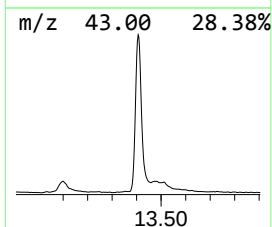
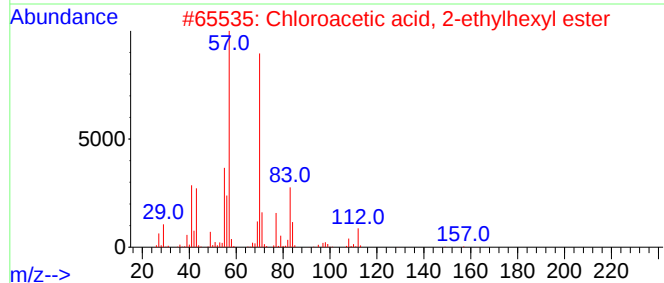
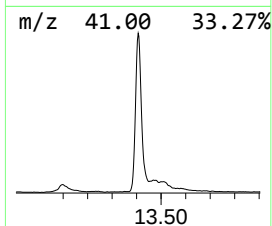
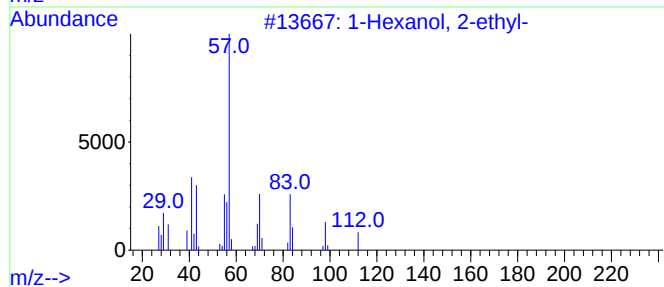
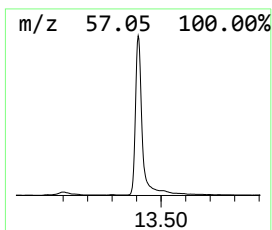
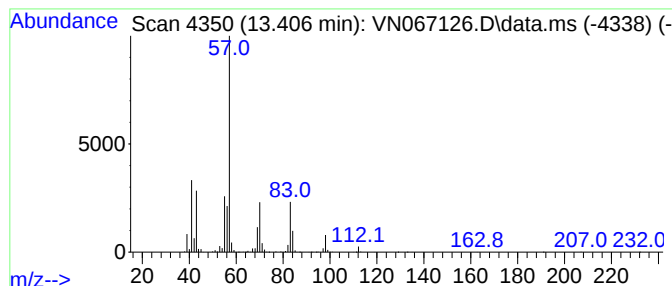
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TIC Integration Parameters: LSCINT.P

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.406	77.58 ug/l	3016270	1,4-Dichlorobenzene-d4	13.299

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	59
3			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	50
4			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
Data File : VN067126.D
Acq On : 18 May 2021 14:52
Operator : JC/MD
Sample : M2387-06 20X
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
41799

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	2.303	38.8	ug/l	1288270	1	7.597	1659430	50.0
2,3-Butanedione	6.567	8.5	ug/l	281897	1	7.597	1659430	50.0
1,3-Dioxane, 2-...	8.780	20.6	ug/l	7806200	2	8.525	18915500	50.0
unknown11.928	11.928	7.0	ug/l	299259	3	11.357	2151980	50.0
3-Dodecene, (E)-	13.098	6.4	ug/l	247603	4	13.299	1943880	50.0
1-Hexanol, 2-et...	13.406	77.6	ug/l	3016270	4	13.299	1943880	50.0