

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051821\
 Data File : VN067130.D
 Acq On : 18 May 2021 16:27
 Operator : JC/MD
 Sample : M2387-10
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 30795

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: VN067130.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.359	535	604	606	rBV2	11584761	81065514	100.00%	66.100%
2	4.033	833	855	911	rVB	1534053	4412399	5.44%	3.598%
3	5.974	1553	1579	1632	rBV2	321152	1106790	1.37%	0.902%
4	6.851	1885	1906	1956	rVB	1498995	4241210	5.23%	3.458%
5	7.519	2131	2155	2168	rBV	372964	928880	1.15%	0.757%
6	7.594	2169	2183	2215	rVB	674406	1659356	2.05%	1.353%
7	7.959	2299	2319	2355	rBV	413699	1013641	1.25%	0.827%
8	8.525	2507	2530	2573	rBV	898479	1941910	2.40%	1.583%
9	8.734	2590	2608	2661	rBV	2184345	4754184	5.86%	3.876%
10	10.035	3077	3093	3106	rVV	1555640	2838534	3.50%	2.315%
11	10.099	3106	3117	3149	rVB	882804	1703627	2.10%	1.389%
12	11.357	3570	3586	3619	rBV	1198887	2193042	2.71%	1.788%
13	11.781	3737	3744	3779	rVV3	288443	905278	1.12%	0.738%
14	12.355	3943	3958	3985	rBV	1071701	1879781	2.32%	1.533%
15	13.296	4297	4309	4324	rBV	1116387	1906217	2.35%	1.554%
16	13.403	4338	4349	4381	rVB	3748286	6453660	7.96%	5.262%
17	13.782	4476	4490	4530	rBV	1510966	3637201	4.49%	2.966%

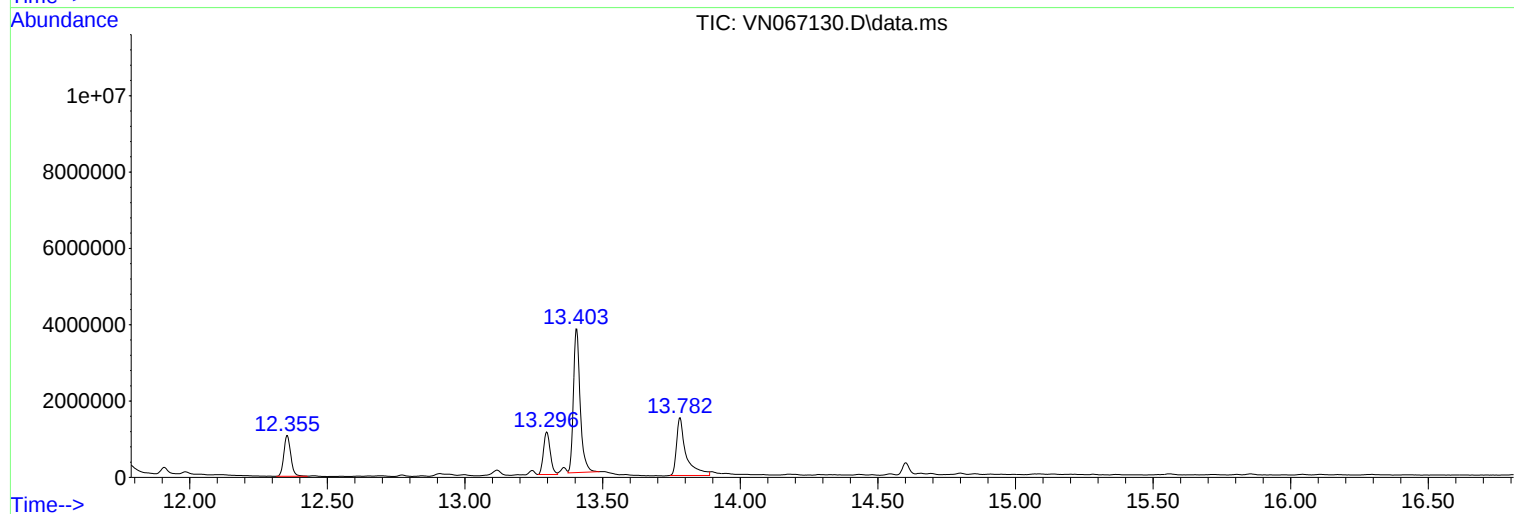
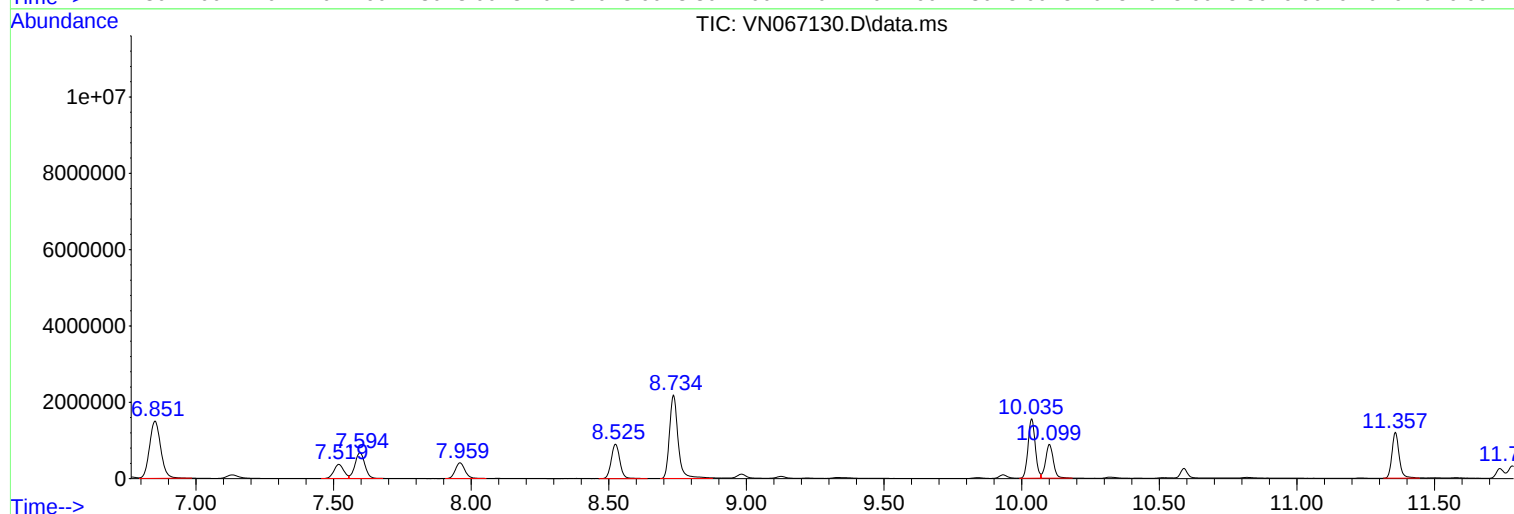
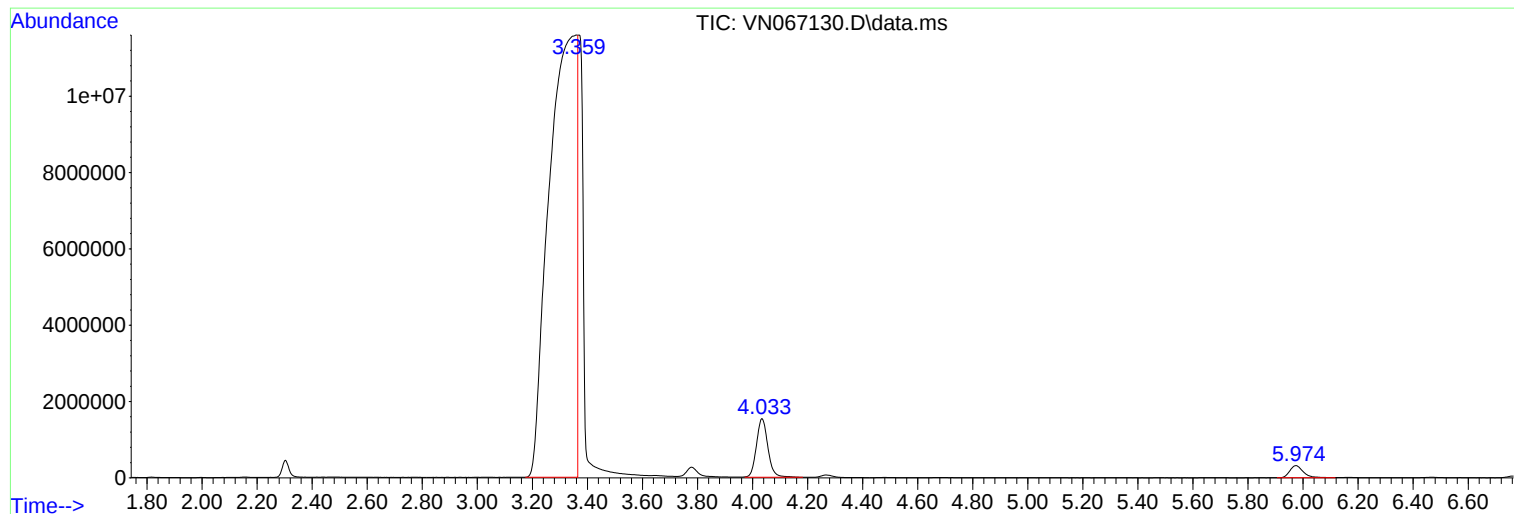
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Quant Title : SW846 8260

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



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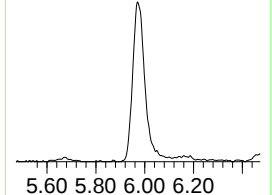
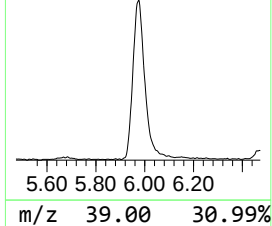
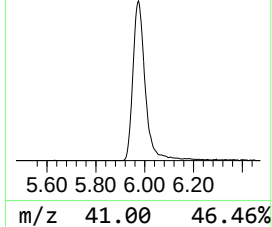
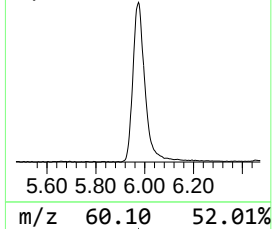
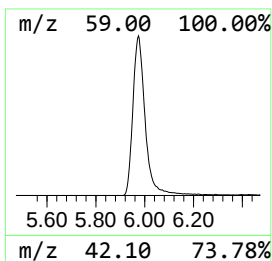
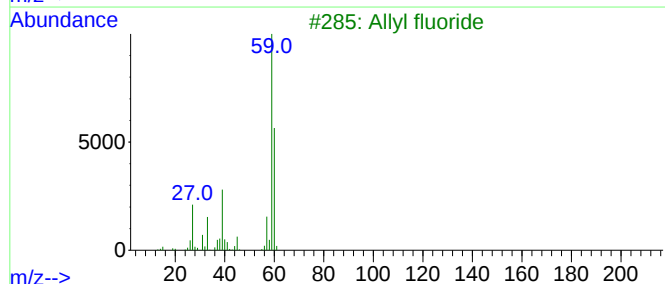
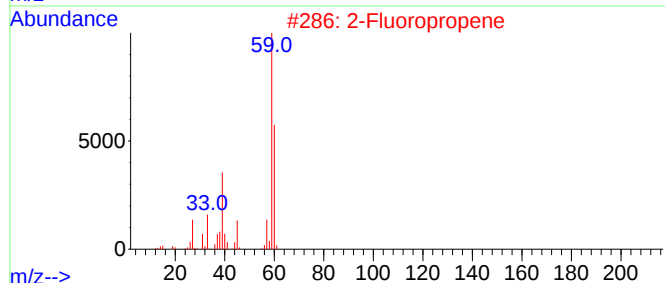
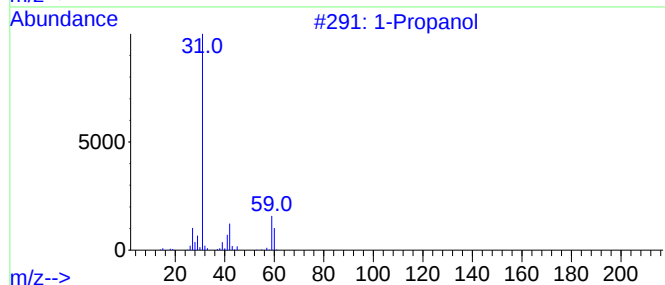
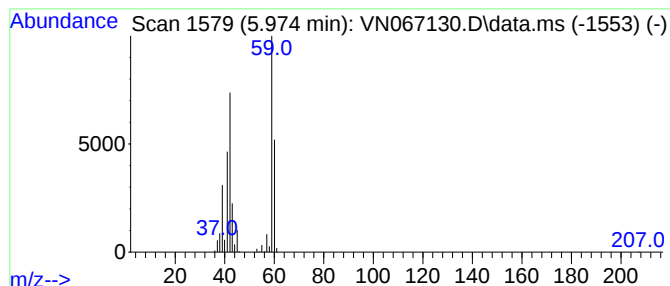
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 2 1-Propanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.974	33.35 ug/l	1106790	Pentafluorobenzene	7.597

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	43
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	25
5			Acetaldoxime	59	C2H5NO	000107-29-9	7



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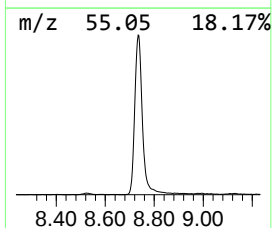
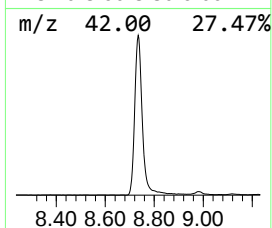
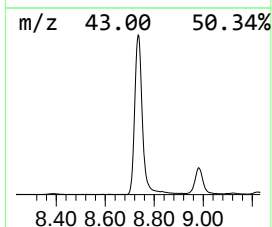
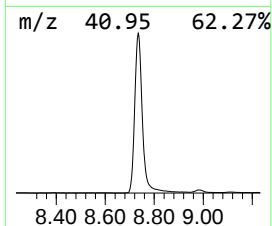
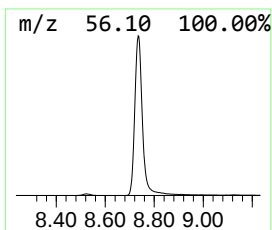
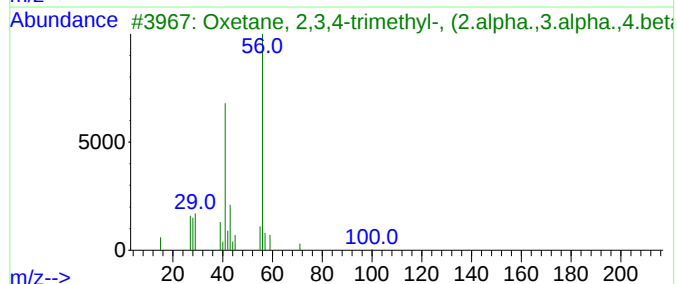
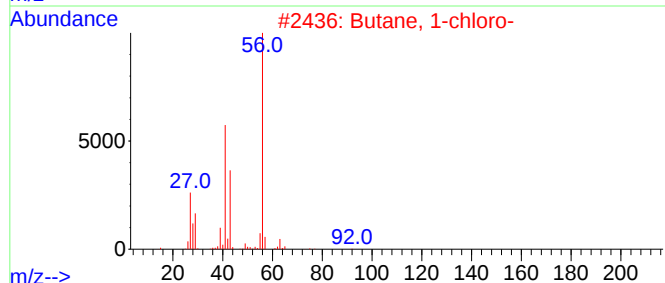
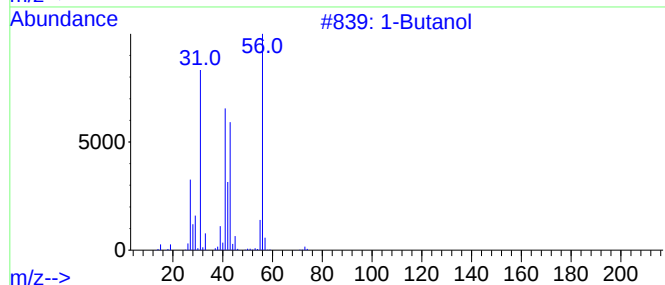
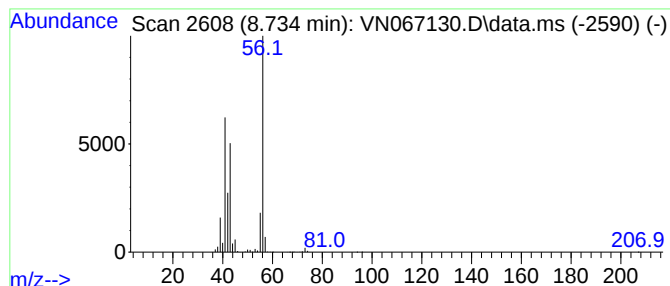
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051421W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Butanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.734	122.41 ug/l	4754180	1,4-Difluorobenzene	8.525

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	91
2			Butane, 1-chloro-	92	C4H9Cl	000109-69-3	45
3			Oxetane, 2,3,4-trimethyl-, (2.alpha...	100	C6H12O	032347-12-9	38
4			Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	36
5			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



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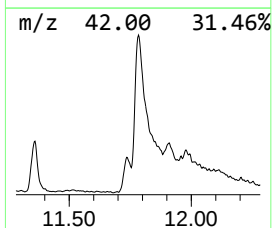
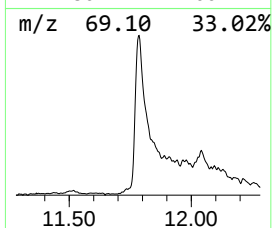
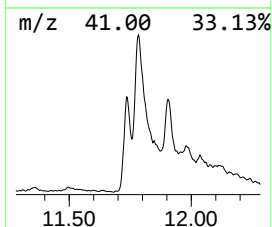
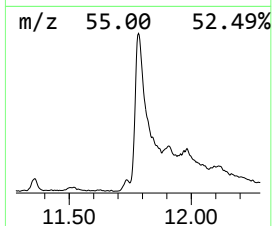
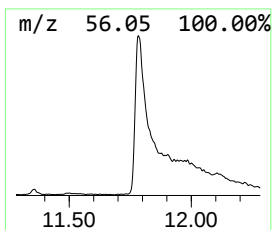
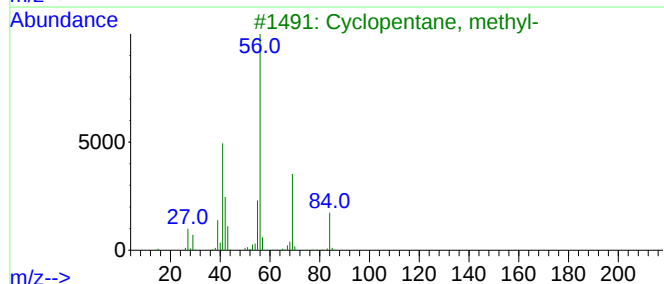
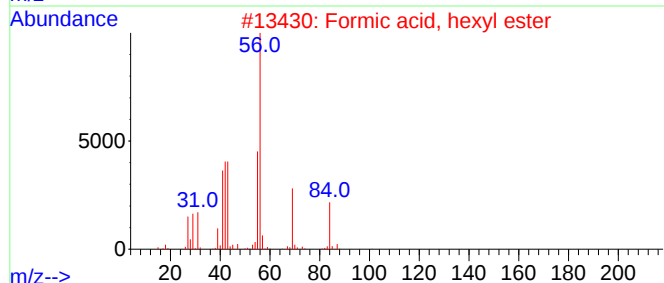
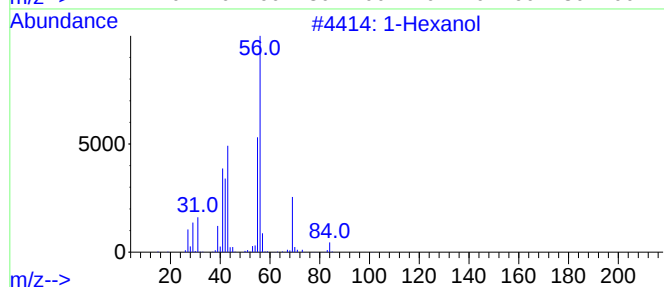
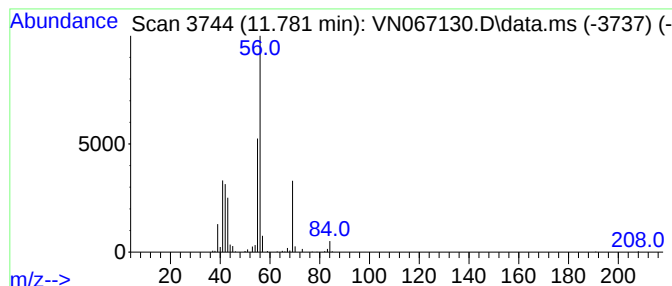
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.781	20.64 ug/l	905278	Chlorobenzene-d5	11.357

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol		102	C6H14O	000111-27-3	72
2	Formic acid, hexyl ester		130	C7H14O2	000629-33-4	64
3	Cyclopentane, methyl-		84	C6H12	000096-37-7	64
4	Cyclopropane, propyl-		84	C6H12	002415-72-7	59
5	1-Pentanol, 4-methyl-		102	C6H14O	000626-89-1	50



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ALS Vial : 14 Sample Multiplier: 1

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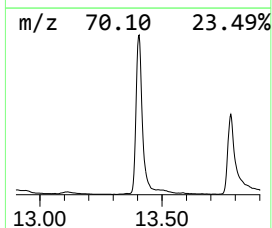
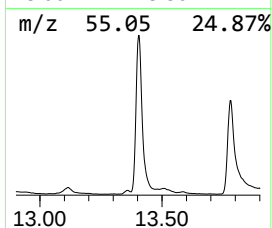
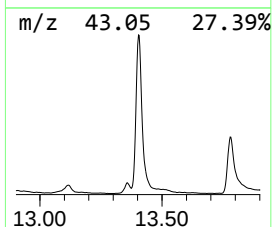
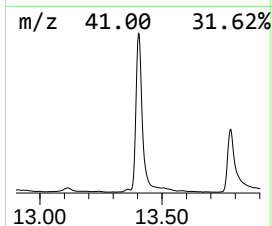
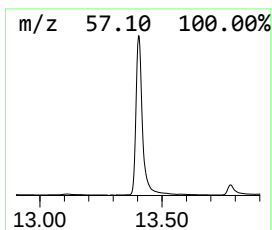
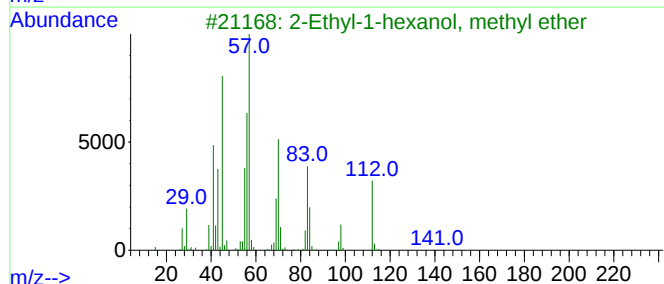
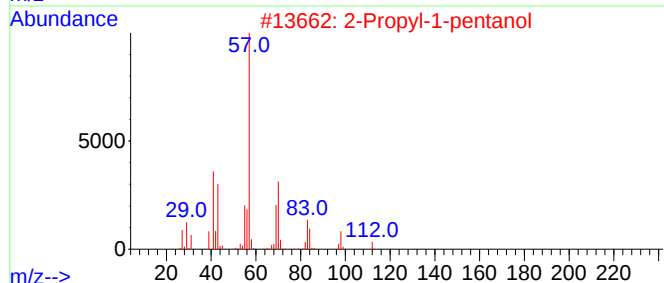
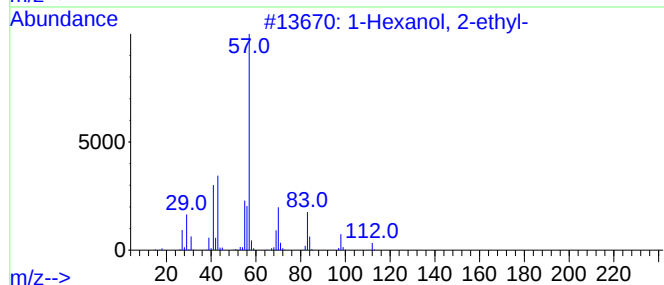
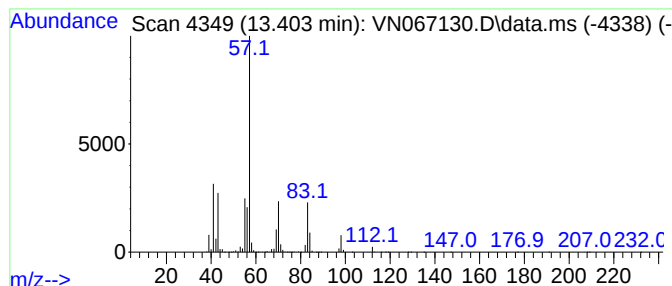
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.403	169.28 ug/l	6453660	1,4-Dichlorobenzene-d4	13.296

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	50
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	40
5			Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	40



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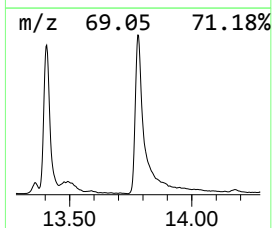
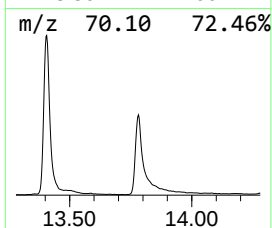
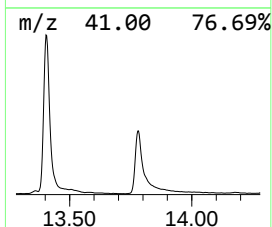
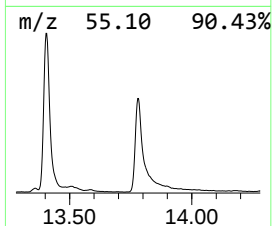
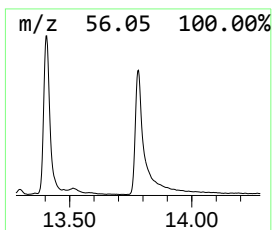
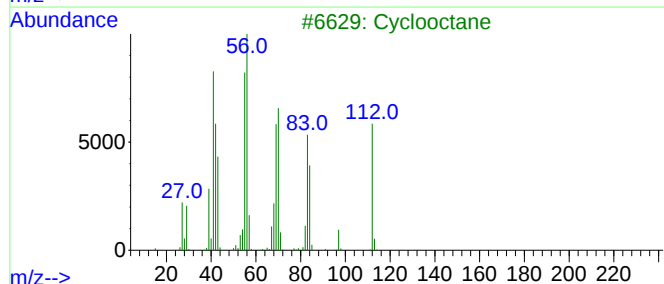
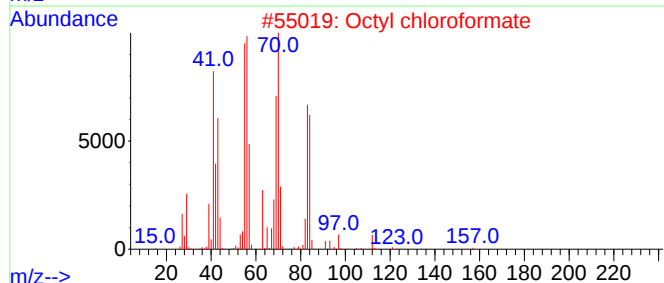
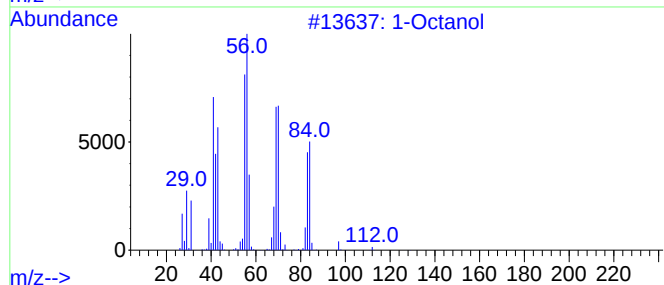
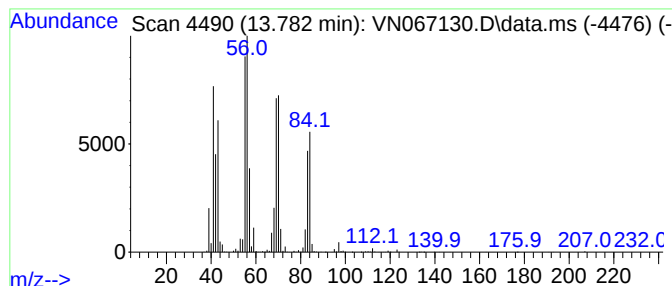
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Quant Title : SW846 8260

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

Peak Number 6 1-Octanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.781	95.40 ug/l	3637200	1,4-Dichlorobenzene-d4	13.296

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Octanol	130	C8H18O	000111-87-5	91
2			Octyl chloroformate	192	C9H17ClO2	007452-59-7	86
3			Cyclooctane	112	C8H16	000292-64-8	74
4			Formic acid, octyl ester	158	C9H18O2	000112-32-3	64
5			1-Octyl trifluoroacetate	226	C10H17F3O2	002561-21-9	59



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	5.974	33.4	ug/l	1106790	1	7.597	1659360	50.0
1-Butanol	8.734	122.4	ug/l	4754180	2	8.525	1941910	50.0
1-Hexanol	11.781	20.6	ug/l	905278	3	11.357	2193040	50.0
1-Hexanol, 2-et...	13.403	169.3	ug/l	6453660	4	13.296	1906220	50.0
1-Octanol	13.781	95.4	ug/l	3637200	4	13.296	1906220	50.0