

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032223\
 Data File : VX034675.D
 Acq On : 22 Mar 2023 16:23
 Operator : JC/MD
 Sample : 02034-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 GW-CB05-20-25-032123

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_X\Method\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.142	6	9	19	rVB	113869	109968	6.14%	0.831%
2	1.258	25	28	33	rBV2	17802	24102	1.35%	0.182%
3	1.355	40	44	51	rBV3	41800	58607	3.27%	0.443%
4	1.453	56	60	64	rVV	32180	36067	2.01%	0.273%
5	1.953	137	142	147	rVB	24906	36210	2.02%	0.274%
6	2.056	154	159	166	rBV	12969	20615	1.15%	0.156%
7	2.136	166	172	182	rVB5	15745	32750	1.83%	0.247%
8	2.294	192	198	207	rVB2	15506	30827	1.72%	0.233%
9	2.380	207	212	224	rVB	41697	70965	3.96%	0.536%
10	2.788	273	279	289	rVB	15403	28619	1.60%	0.216%
11	3.605	402	413	426	rBV	246912	590508	32.96%	4.462%
12	4.489	549	558	565	rBV2	13315	34929	1.95%	0.264%
13	5.093	639	657	671	rBV	43931	139373	7.78%	1.053%
14	5.385	693	705	721	rBV	199899	585238	32.67%	4.422%
15	5.550	721	732	749	rVB	363642	1031765	57.59%	7.796%
16	5.958	787	799	814	rBV	251238	679395	37.92%	5.134%
17	6.763	921	931	950	rBV	567440	1364648	76.17%	10.311%
18	7.153	986	995	1002	rBV3	12786	33329	1.86%	0.252%
19	7.586	1058	1066	1073	rBV2	19606	42999	2.40%	0.325%
20	7.659	1073	1078	1091	rVB2	19252	42855	2.39%	0.324%
21	8.647	1233	1240	1248	rBV	1136765	1791511	100.00%	13.537%
22	8.720	1248	1252	1260	rVB4	9533	18536	1.03%	0.140%
23	9.519	1378	1383	1401	rBV	454679	632017	35.28%	4.776%
24	10.055	1465	1471	1489	rVB	1165281	1578041	88.08%	11.924%
25	10.585	1553	1558	1573	rBV	124631	270206	15.08%	2.042%
26	10.860	1598	1603	1615	rVB	51679	75812	4.23%	0.573%
27	11.079	1632	1639	1649	rBV	989630	1233429	68.85%	9.320%
28	11.591	1718	1723	1726	rBV	25132	32011	1.79%	0.242%
29	11.658	1731	1734	1741	rVV2	12920	23324	1.30%	0.176%
30	11.927	1774	1778	1788	rBV	55276	78758	4.40%	0.595%
31	12.018	1788	1793	1803	rVB	1129393	1491767	83.27%	11.272%
32	12.219	1822	1826	1836	rBV3	14736	35716	1.99%	0.270%
33	12.591	1882	1887	1900	rBV2	41388	100857	5.63%	0.762%
34	12.859	1925	1931	1947	rBV	286244	409768	22.87%	3.096%
35	13.426	2018	2024	2041	rBV2	165203	440296	24.58%	3.327%
36	14.262	2156	2161	2176	rVB3	16889	28435	1.59%	0.215%

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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_X\Method\82X031023W.M
Title : SW846 8260

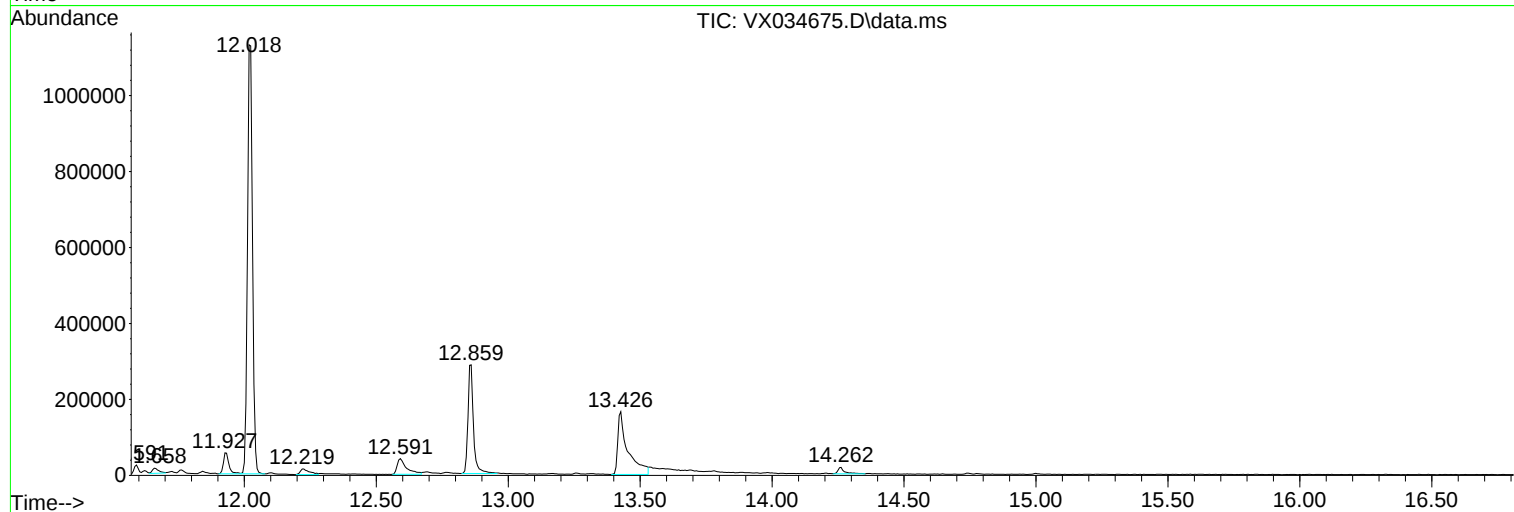
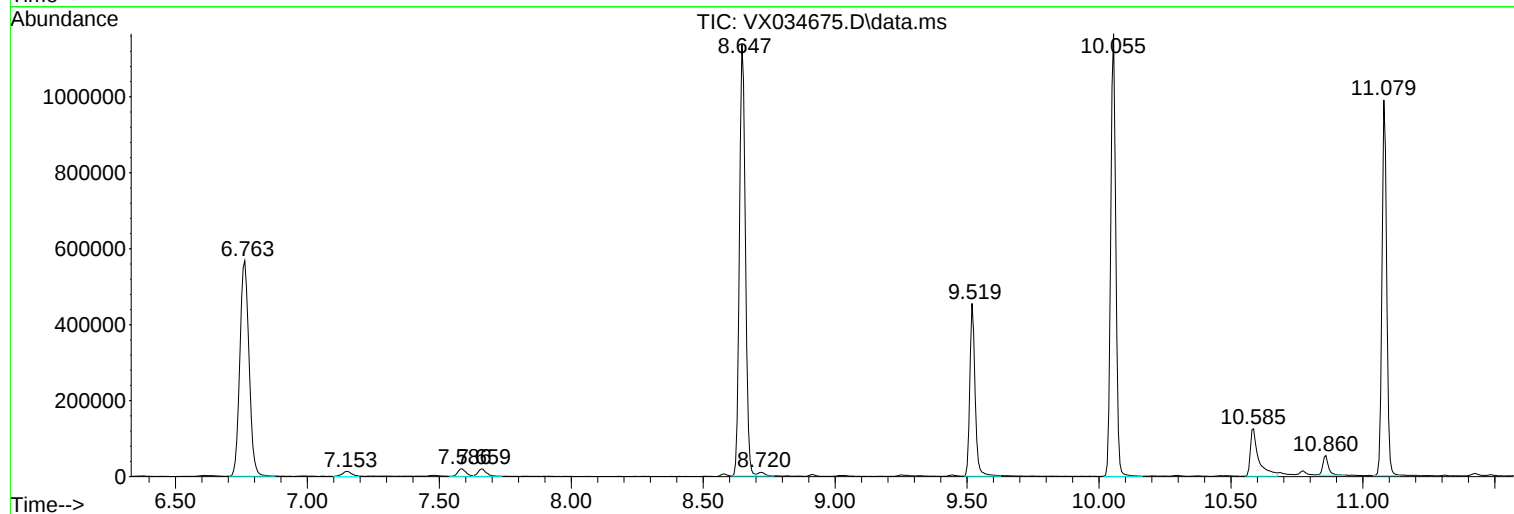
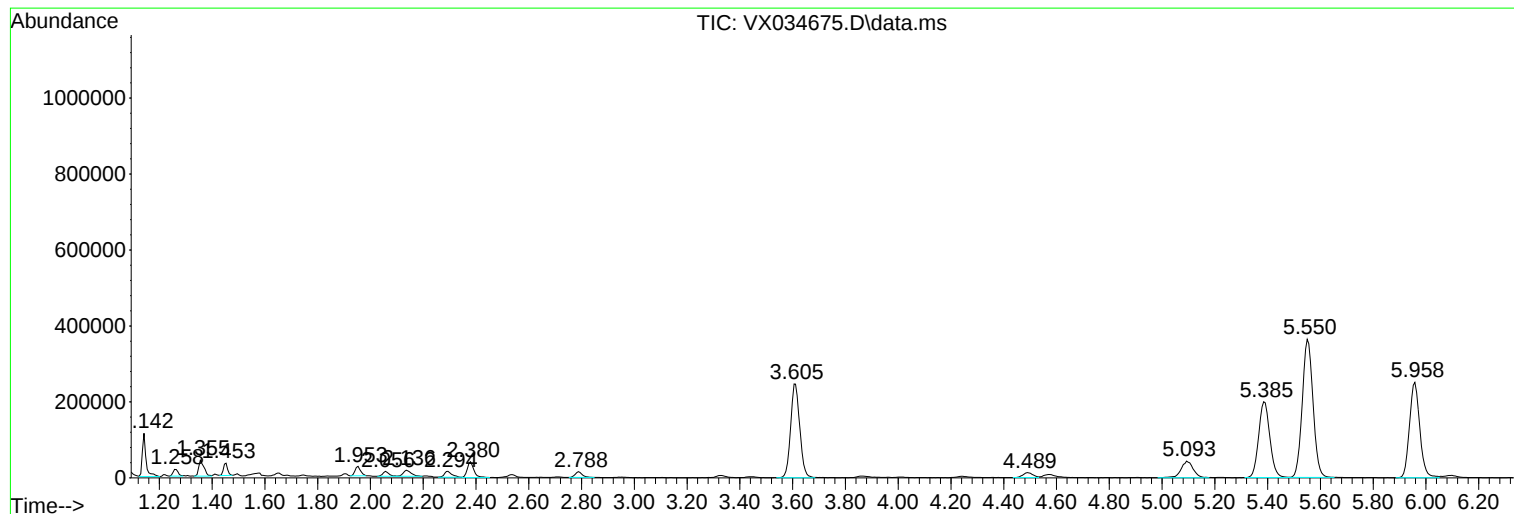
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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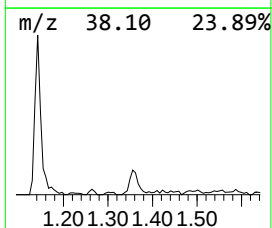
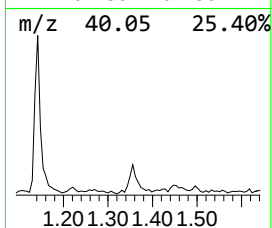
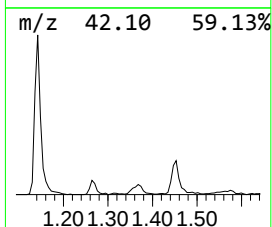
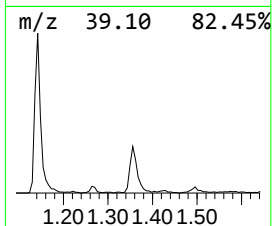
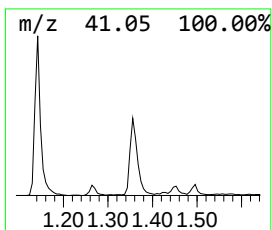
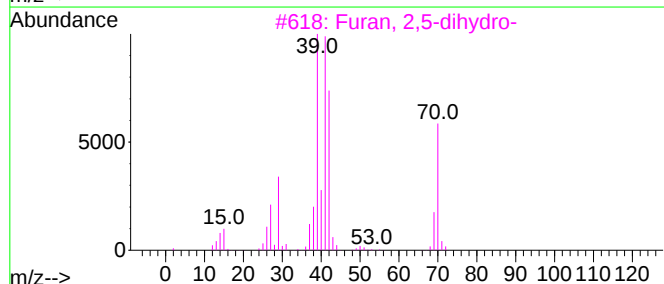
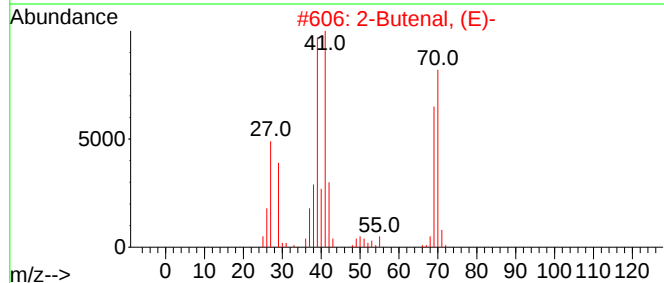
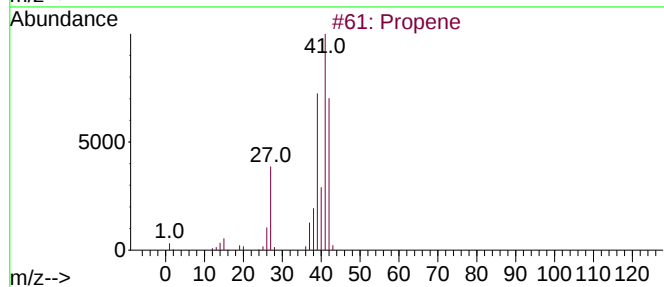
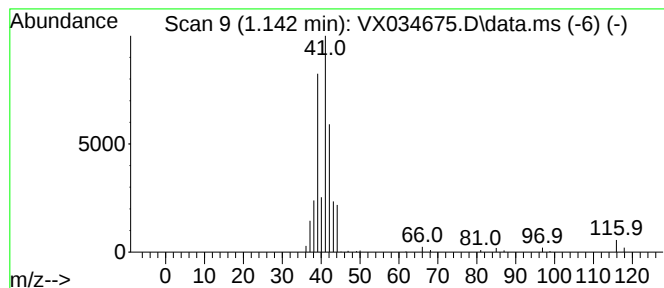
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Propene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.142	5.33 ug/l	109968	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
3			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	64
4			3-Butenoic acid	86	C4H6O2	000625-38-7	64
5			Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	64



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Instrument :
MSVOA_X
ClientSampleId :
GW-CB05-20-25-032123

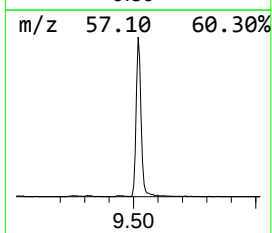
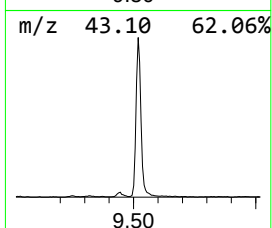
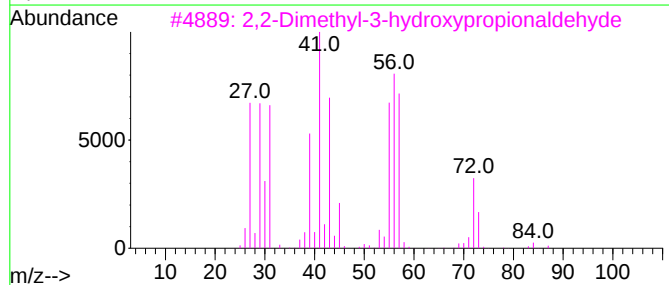
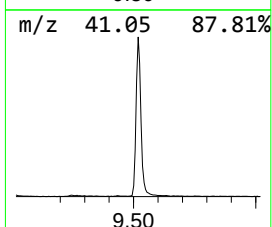
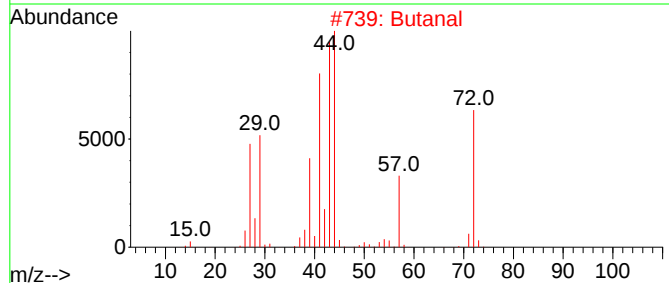
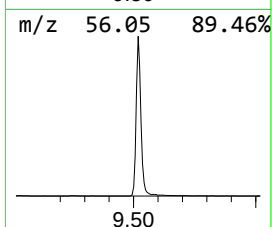
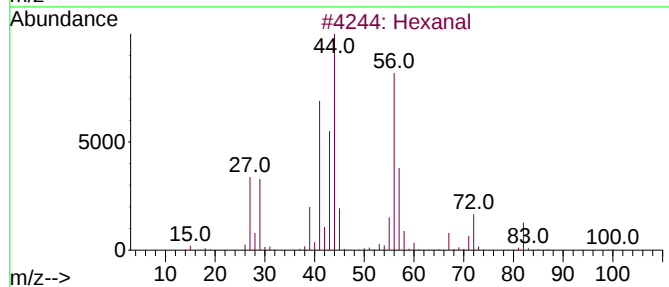
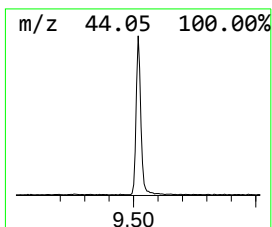
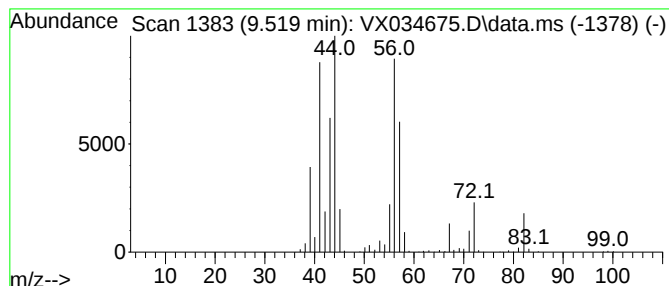
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TIC Library : C:\Database\NIST20.L
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Peak Number 2 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	20.03 ug/l	632017	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	87
2			Butanal	72	C4H8O	000123-72-8	38
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	25
4			1-Propene, 2-methyl-	56	C4H8	000115-11-7	16
5			Aziridine, 2-methyl-	57	C3H7N	000075-55-8	14



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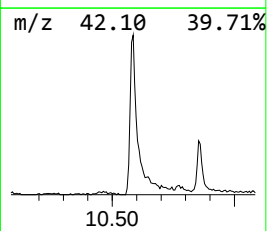
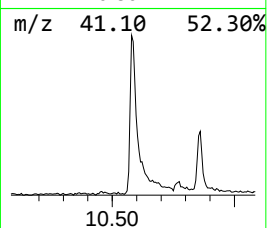
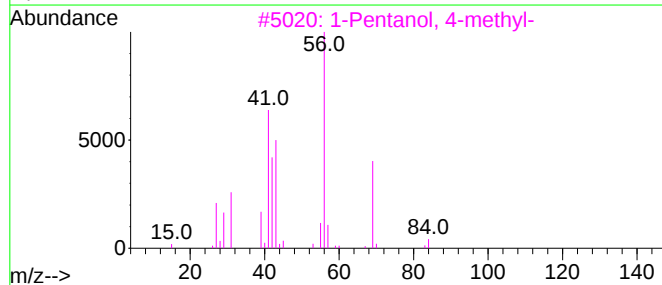
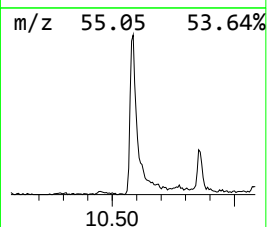
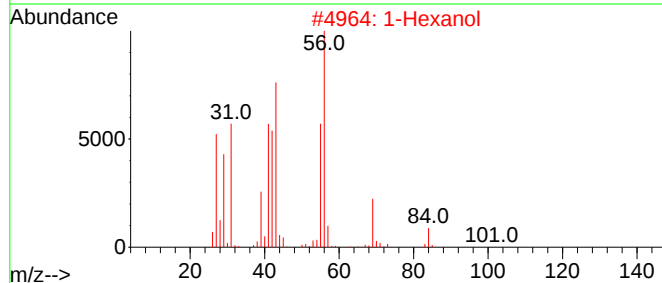
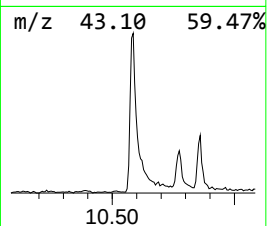
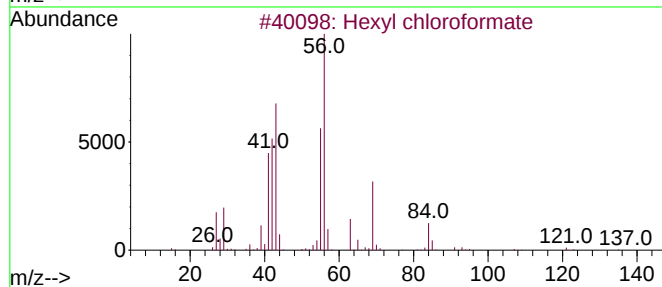
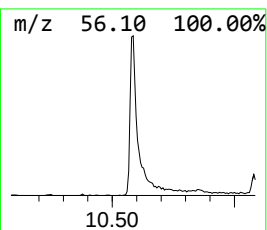
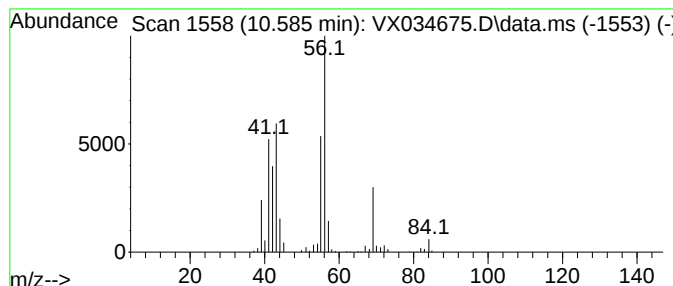
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Hexyl chloroformate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.585	8.56 ug/l	270206	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexyl chloroformate	164	C7H13ClO2	006092-54-2	83
2			1-Hexanol	102	C6H14O	000111-27-3	83
3			1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	72
4			Formic acid, hexyl ester	130	C7H14O2	000629-33-4	72
5			Cyclopropane, propyl-	84	C6H12	002415-72-7	64



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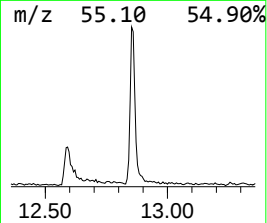
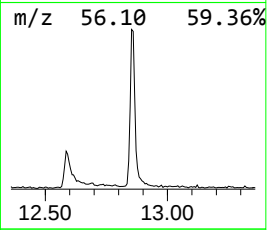
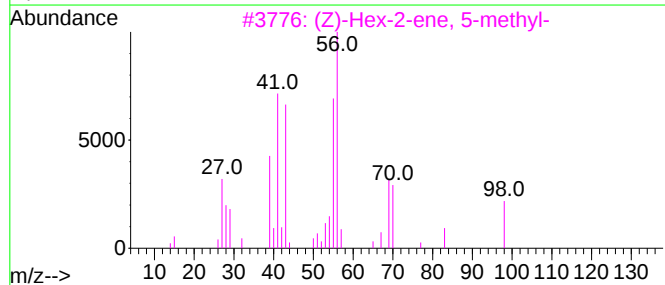
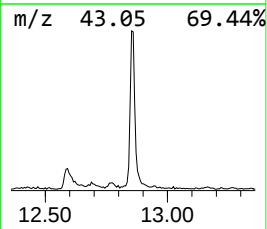
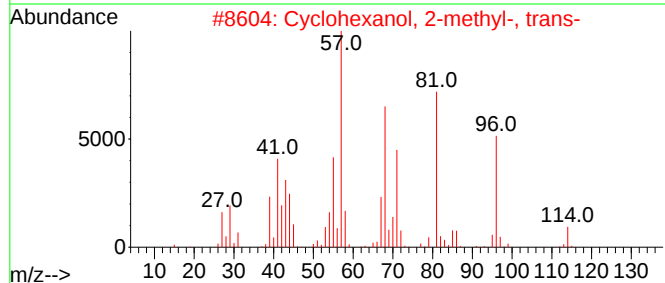
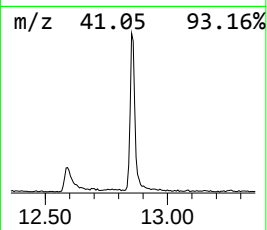
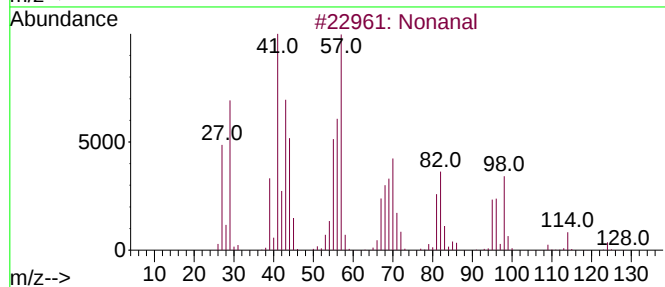
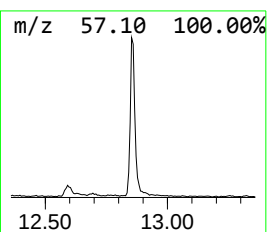
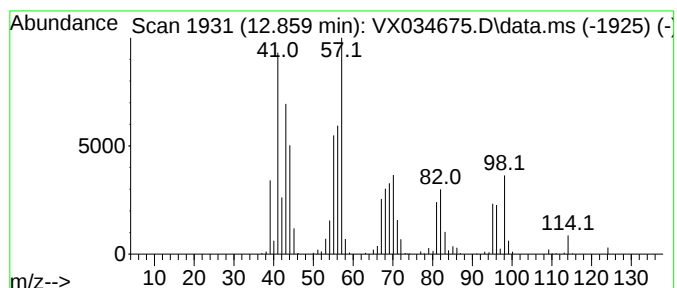
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.859	13.73 ug/l	409768	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	91
2			Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	38
3			(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	22
4			Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	22
5			Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	22



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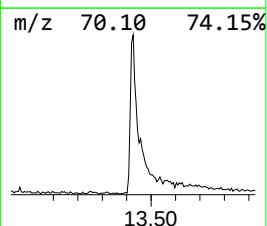
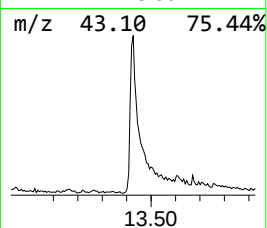
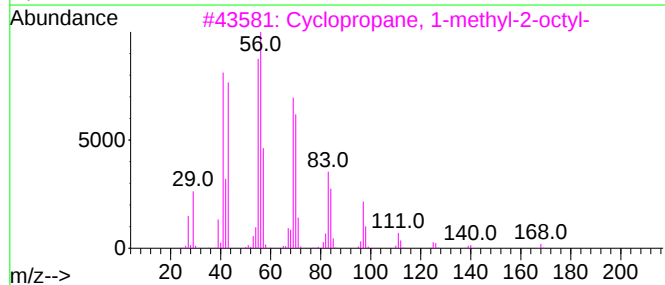
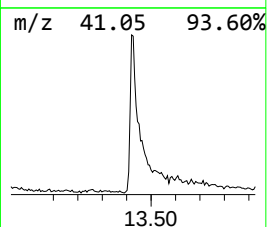
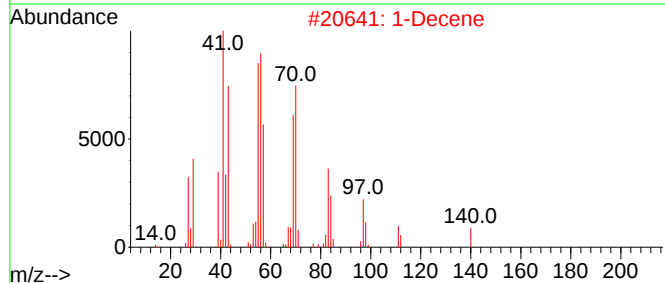
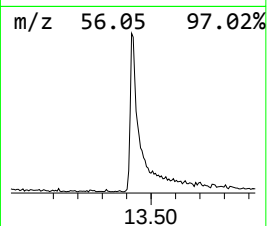
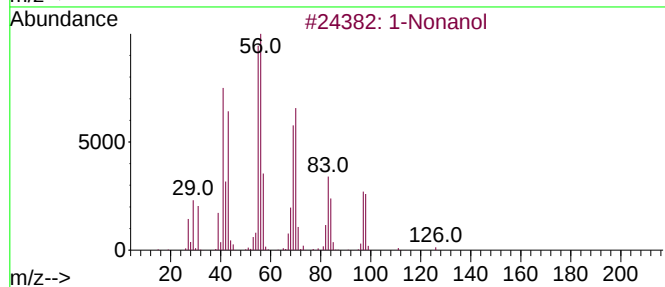
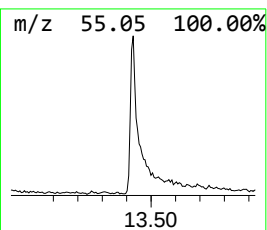
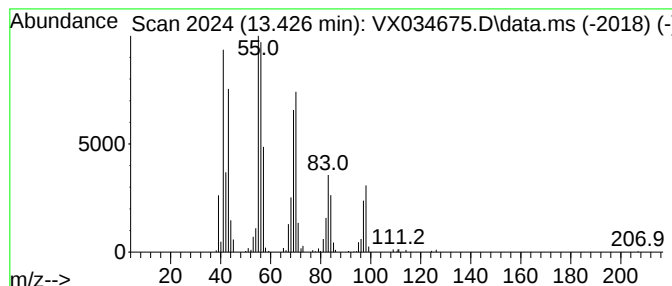
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Nonanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.426	14.76 ug/l	440296	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Nonanol	144	C9H20O	000143-08-8	91
2			1-Decene	140	C10H20	000872-05-9	86
3			Cyclopropane, 1-methyl-2-octyl-	168	C12H24	037617-26-8	86
4			Cyclopropane, 1-ethyl-2-heptyl-	168	C12H24	074663-86-8	80
5			Cycloheptane	98	C7H14	000291-64-5	74



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032223\
Data File : VX034675.D
Acq On : 22 Mar 2023 16:23
Operator : JC/MD
Sample : 02034-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
GW-CB05-20-25-032123

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.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
Propene	1.142	5.3	ug/l	109968	1	5.550	1031770	50.0
Hexanal	9.519	20.0	ug/l	632017	3	10.055	1578040	50.0
Hexyl chlorofo...	10.585	8.6	ug/l	270206	3	10.055	1578040	50.0
Nonanal	12.859	13.7	ug/l	409768	4	12.024	1491770	50.0
1-Nonanol	13.426	14.8	ug/l	440296	4	12.024	1491770	50.0