

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
 Data File : VX039796.D
 Acq On : 17 Jan 2024 12:52
 Operator : JC/MD
 Sample : P1156-04
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SUMOGW-9-23-26

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\82X011024W.M
 Title : SW846 8260

Signal : TIC: VX039796.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	14	rVB2	15114	15029	2.45%	0.360%
2	1.355	42	44	50	rVB2	5537	8186	1.33%	0.196%
3	1.453	56	60	65	rBV	14143	16245	2.65%	0.389%
4	2.288	191	197	204	rBV	6349	10541	1.72%	0.253%
5	2.374	204	211	223	rVB	6118	10913	1.78%	0.262%
6	4.233	508	516	528	rBV5	3890	11594	1.89%	0.278%
7	5.093	644	657	671	rBV	85005	262628	42.81%	6.295%
8	5.385	694	705	720	rBV	67726	199666	32.55%	4.786%
9	5.550	720	732	749	rVV	109811	309896	50.52%	7.428%
10	5.952	789	798	811	rBV	80851	213131	34.74%	5.109%
11	6.757	921	930	947	rBV	183226	439082	71.57%	10.525%
12	7.580	1060	1065	1077	rBV2	6479	13323	2.17%	0.319%
13	8.647	1233	1240	1249	rBV	396377	613468	100.00%	14.705%
14	9.519	1377	1383	1400	rBV	102462	144923	23.62%	3.474%
15	10.049	1465	1470	1481	rBV	406073	569961	92.91%	13.662%
16	10.854	1597	1602	1618	rBV2	93120	117998	19.23%	2.828%
17	11.079	1634	1639	1652	rBV	352082	452287	73.73%	10.841%
18	11.902	1768	1774	1775	rBV3	6078	7478	1.22%	0.179%
19	11.927	1775	1778	1781	rVB2	12151	13222	2.16%	0.317%
20	12.018	1786	1793	1803	rVB	466124	605809	98.75%	14.521%
21	12.195	1817	1822	1828	rBV4	4327	7398	1.21%	0.177%
22	12.256	1828	1832	1838	rVB3	4284	6325	1.03%	0.152%
23	12.853	1925	1930	1938	rBV	52677	64866	10.57%	1.555%
24	13.463	2026	2030	2042	rVB2	42173	57853	9.43%	1.387%

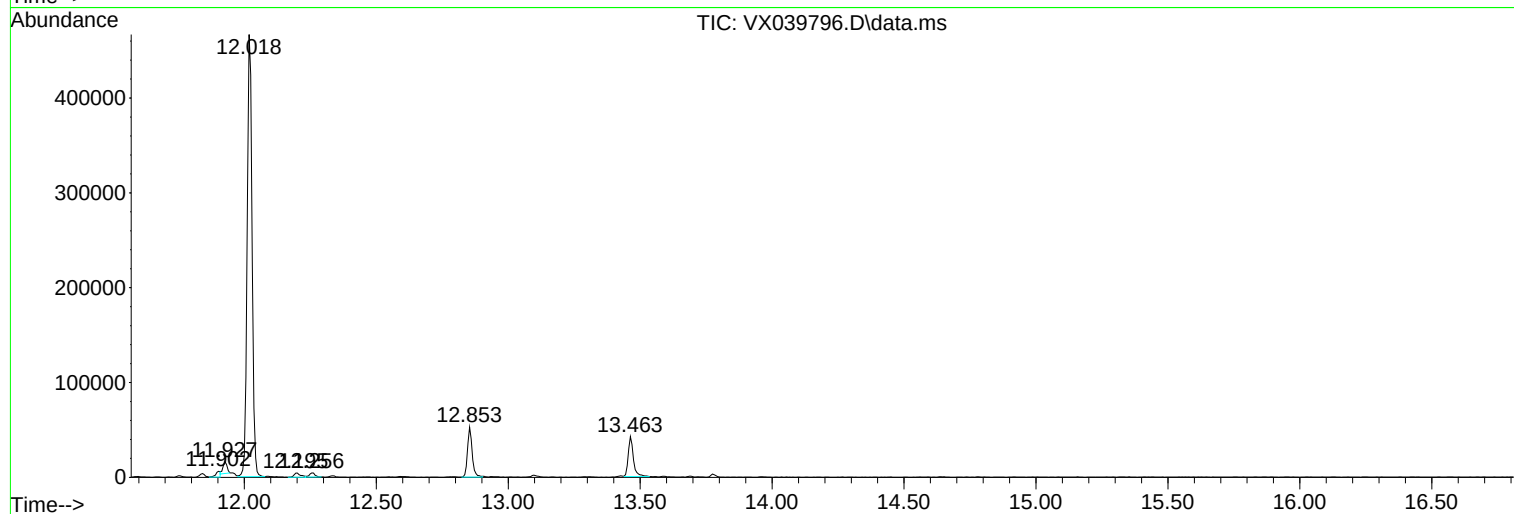
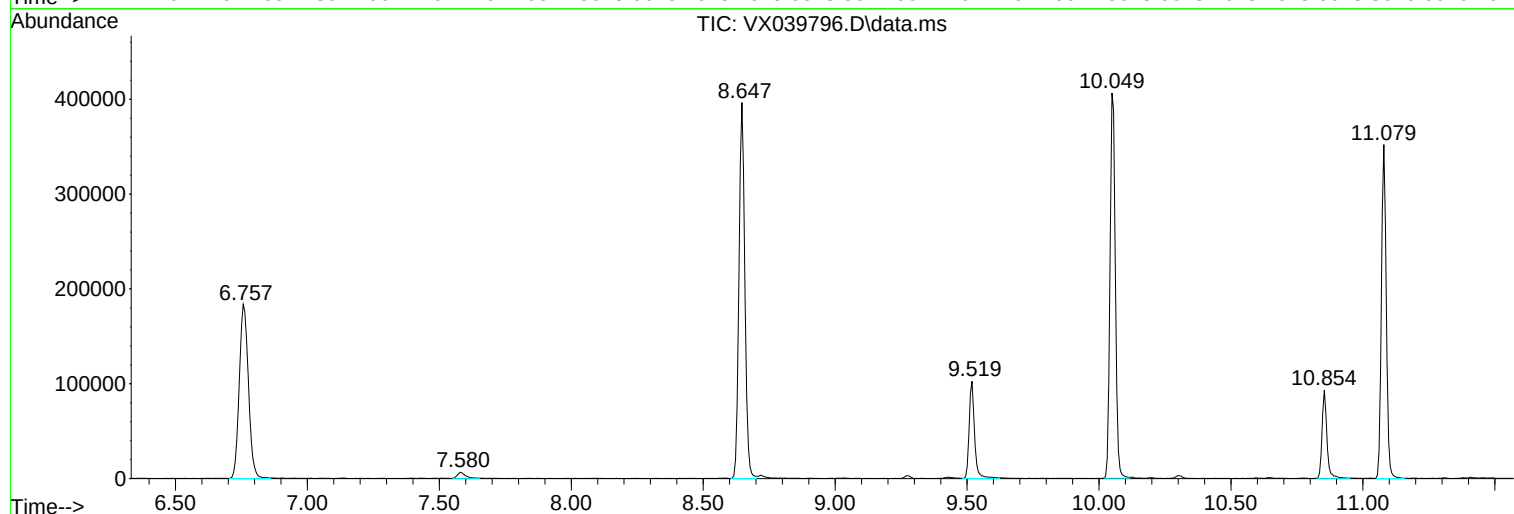
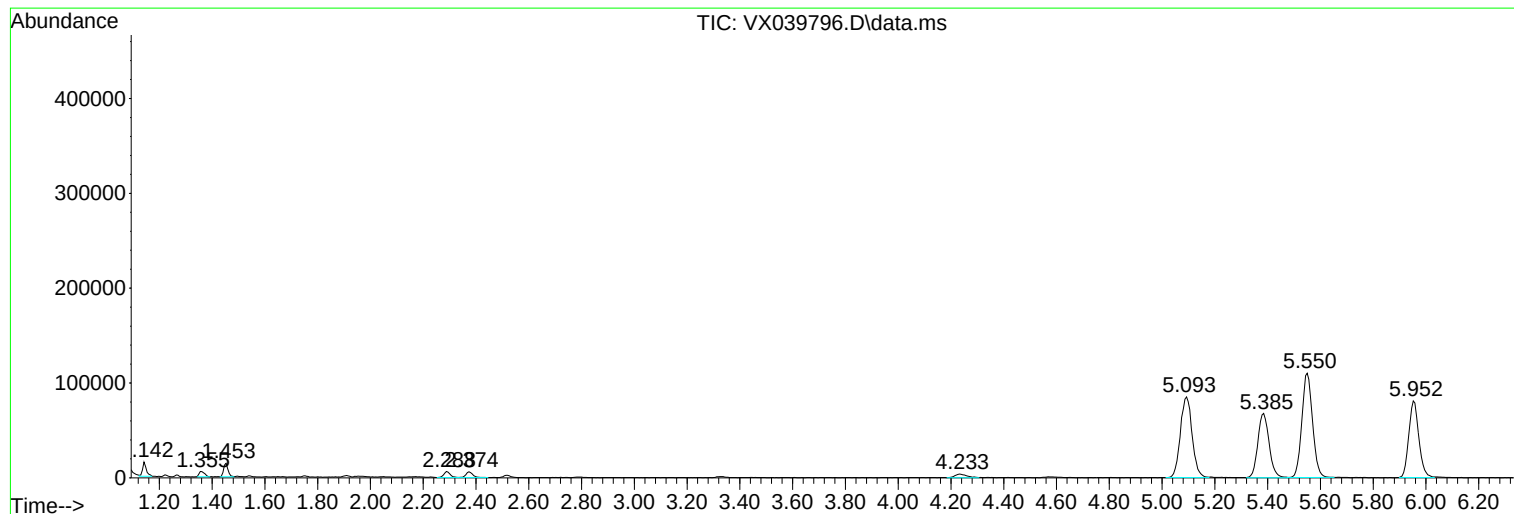
Sum of corrected areas: 4171822

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
Data File : VX039796.D
Acq On : 17 Jan 2024 12:52
Operator : JC/MD
Sample : P1156-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SUMOGW-9-23-26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
Data File : VX039796.D
Acq On : 17 Jan 2024 12:52
Operator : JC/MD
Sample : P1156-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SUMOGW-9-23-26

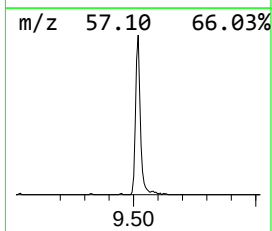
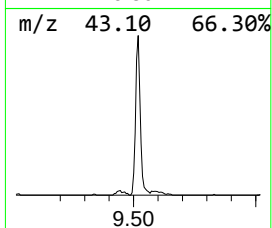
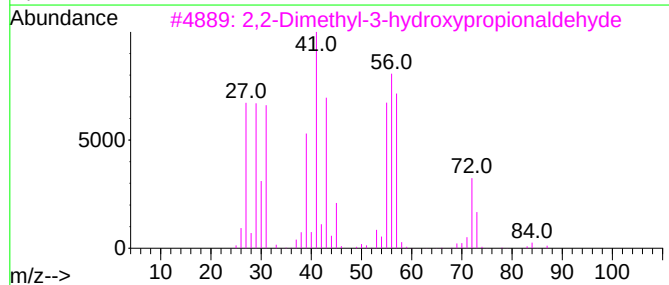
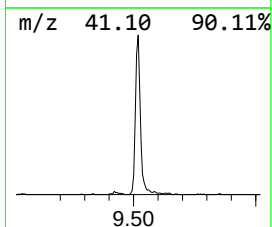
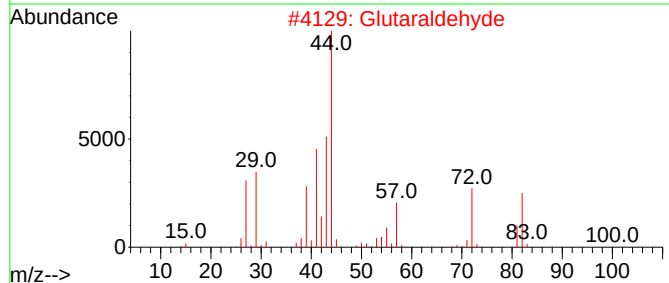
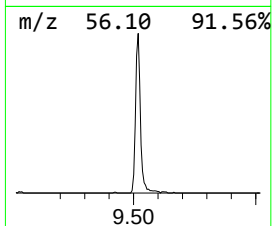
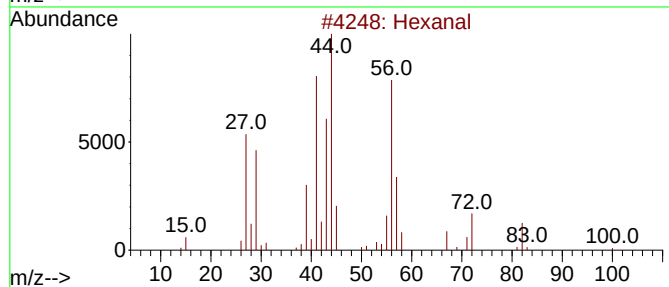
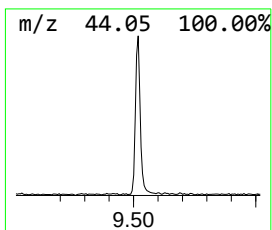
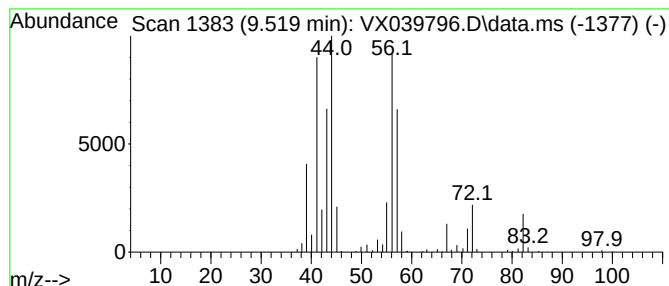
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.519	12.71 ug/l	144923	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	80
2			Glutaraldehyde	100	C5H8O2	000111-30-8	30
3			2,2-Dimethyl-3-hydroxypropionald...	102	C5H10O2	000597-31-9	23
4			Butanal	72	C4H8O	000123-72-8	16
5			Butanal, 3-methyl-	86	C5H10O	000590-86-3	16



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
Data File : VX039796.D
Acq On : 17 Jan 2024 12:52
Operator : JC/MD
Sample : P1156-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SUMOGW-9-23-26

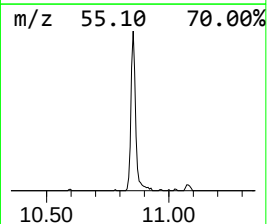
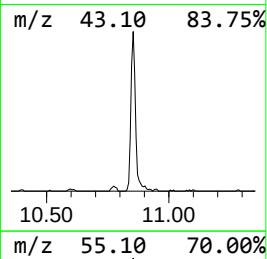
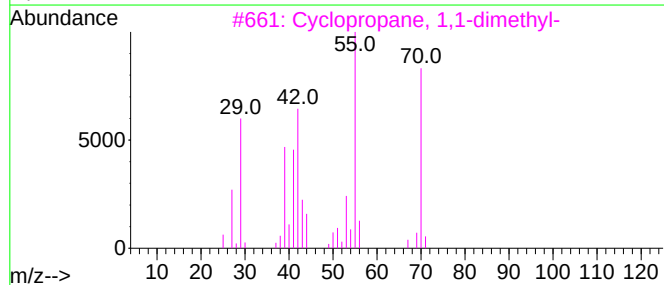
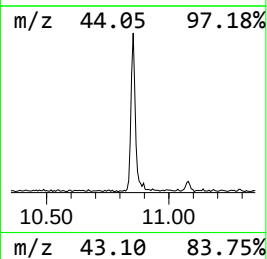
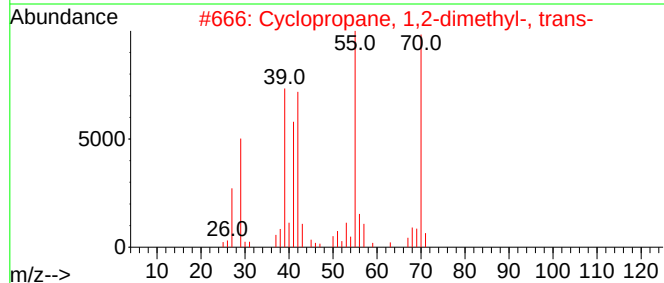
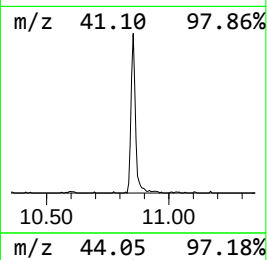
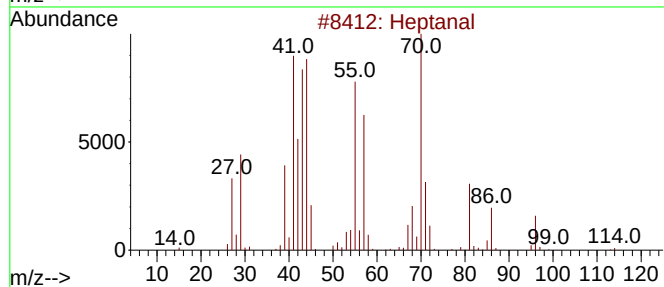
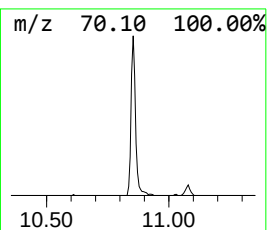
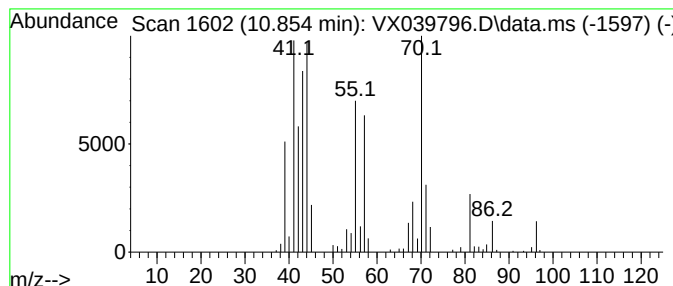
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 2 Heptanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.854	10.35 ug/l	117998	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanal	114	C7H14O	000111-71-7	90
2			Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	43
3			Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	32
4			Oxirane, 2-(1,1-dimethylethyl)-3...	114	C7H14O	053897-30-6	32
5			2-Methyl-1-butene	70	C5H10	000563-46-2	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
Data File : VX039796.D
Acq On : 17 Jan 2024 12:52
Operator : JC/MD
Sample : P1156-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SUMOGW-9-23-26

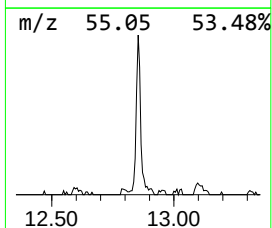
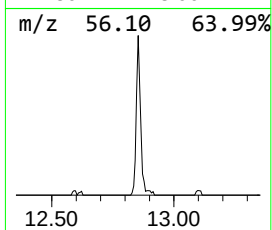
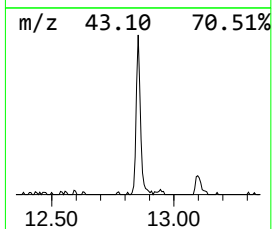
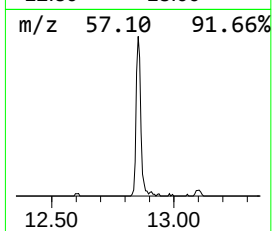
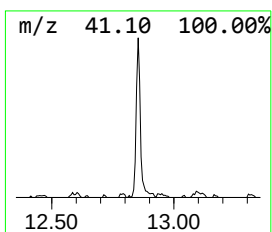
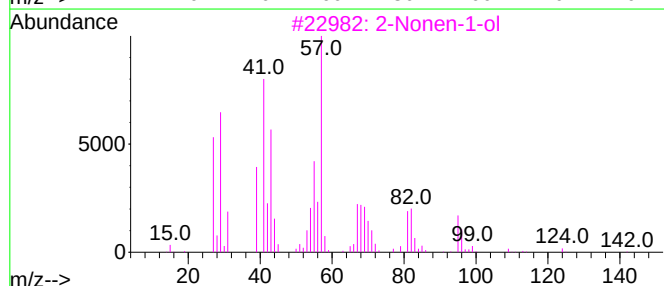
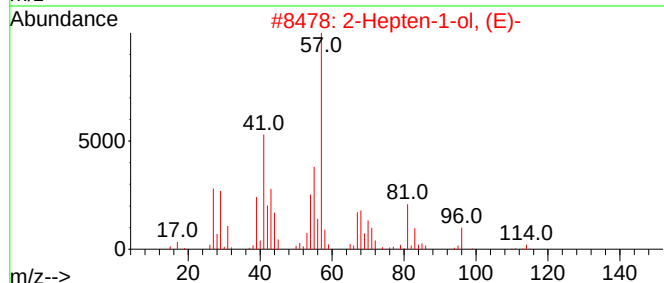
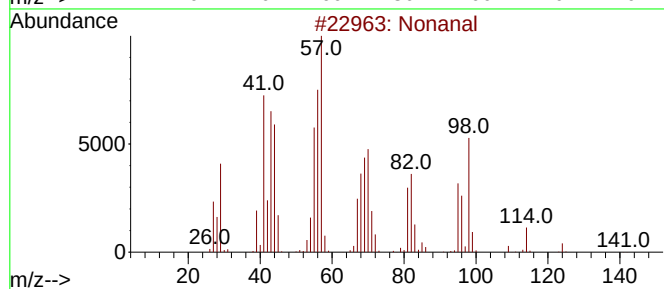
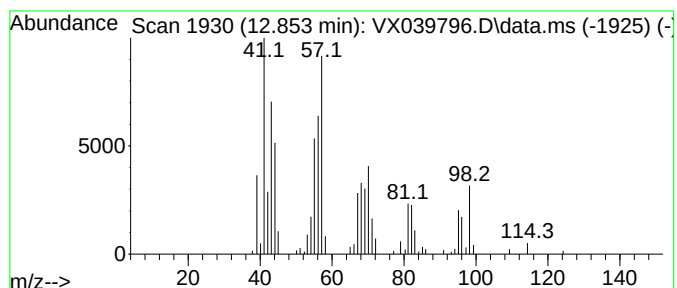
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

Peak Number 3 Nonanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.853	5.35 ug/l	64866	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonanal	142	C9H18O	000124-19-6	83
2			2-Hepten-1-ol, (E)-	114	C7H14O	033467-76-4	38
3			2-Nonen-1-ol	142	C9H18O	022104-79-6	35
4			Cycloheptane	98	C7H14	000291-64-5	35
5			2-Propen-1-amine, N-2-propenyl-	97	C6H11N	000124-02-7	27



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX011724\
Data File : VX039796.D
Acq On : 17 Jan 2024 12:52
Operator : JC/MD
Sample : P1156-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SUMOGW-9-23-26

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X011024W.M
Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexanal	9.519	12.7	ug/l	144923	3	10.055	569961	50.0
Heptanal	10.854	10.4	ug/l	117998	3	10.055	569961	50.0
Nonanal	12.853	5.3	ug/l	64866	4	12.024	605809	50.0