

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
 Data File : VX026273.D
 Acq On : 04 Jan 2022 15:51
 Operator : JC/MD
 Sample : M5328-10
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 20995

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\82X123021W.M
 Title : SW846 8260

Signal : TIC: VX026273.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	56	59	90	rVB	9667795	13259518	100.00%	43.932%
2	2.063	152	160	186	rVB	992506	1719578	12.97%	5.697%
3	2.294	192	198	207	rBV	2470265	4005080	30.21%	13.270%
4	2.380	207	212	230	rVB	342179	579809	4.37%	1.921%
5	3.843	436	452	470	rBV2	51955	156190	1.18%	0.517%
6	4.227	503	515	534	rBV	140755	387429	2.92%	1.284%
7	4.556	557	569	581	rBV	589372	1656742	12.49%	5.489%
8	4.995	626	641	666	rBV	192956	631450	4.76%	2.092%
9	5.391	695	706	722	rVB2	99705	288014	2.17%	0.954%
10	5.556	722	733	747	rBV	172816	487681	3.68%	1.616%
11	5.958	788	799	809	rBV	117955	313989	2.37%	1.040%
12	6.763	919	931	947	rVB	273691	652041	4.92%	2.160%
13	7.208	996	1004	1024	rBV	113053	249248	1.88%	0.826%
14	8.653	1234	1241	1249	rBV	531622	894876	6.75%	2.965%
15	9.494	1373	1379	1395	rBV2	84313	193900	1.46%	0.642%
16	10.055	1465	1471	1482	rVB	550001	763423	5.76%	2.529%
17	10.153	1482	1487	1500	rBV	279045	377055	2.84%	1.249%
18	10.756	1581	1586	1594	rBV	102957	165073	1.24%	0.547%
19	11.079	1634	1639	1646	rBV	453997	613426	4.63%	2.032%
20	12.024	1789	1794	1800	rVB	569412	717351	5.41%	2.377%
21	12.219	1821	1826	1838	rBV	1499882	1873227	14.13%	6.206%
22	12.421	1854	1859	1864	rVB2	157575	196643	1.48%	0.652%

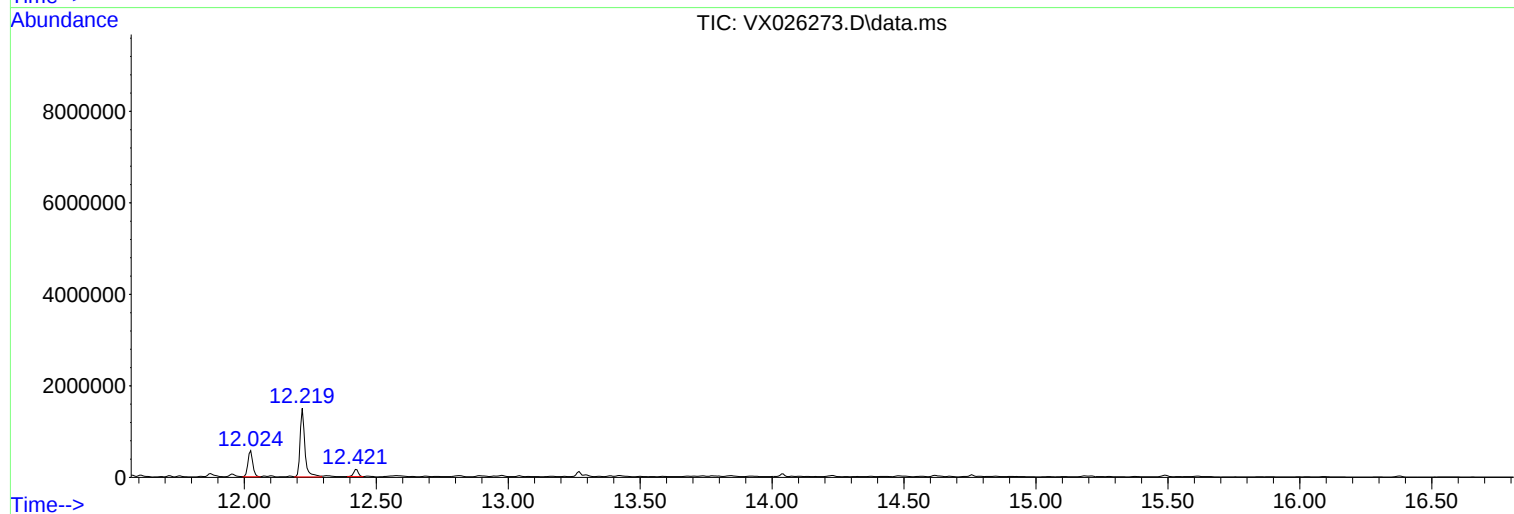
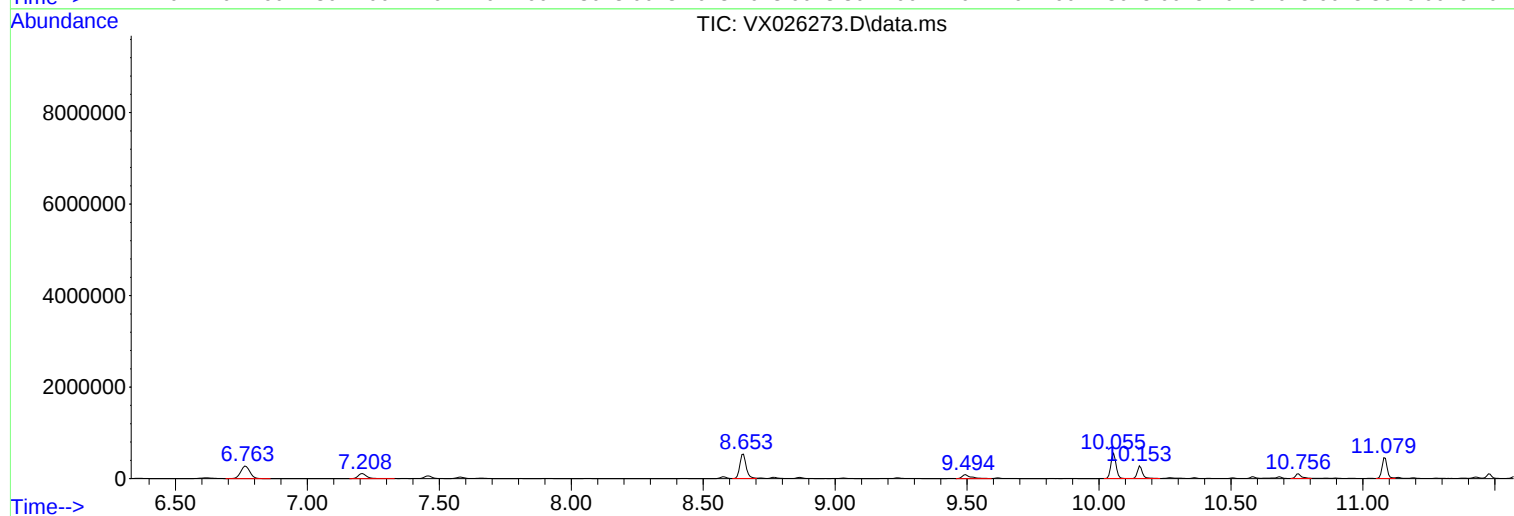
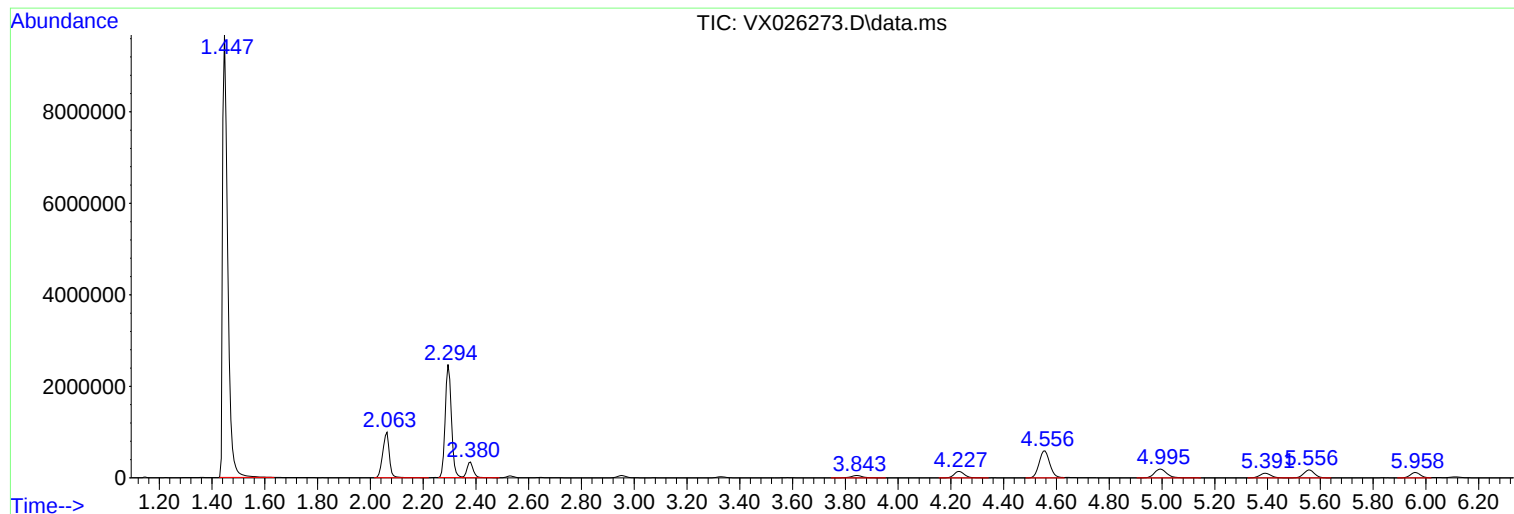
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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



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20995

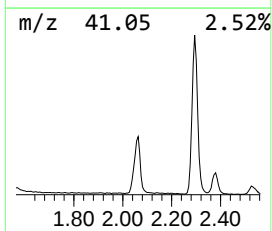
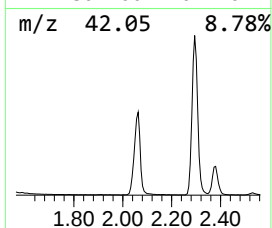
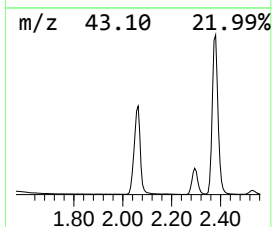
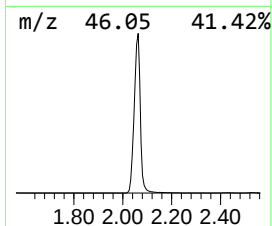
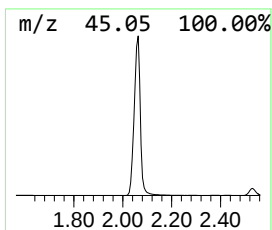
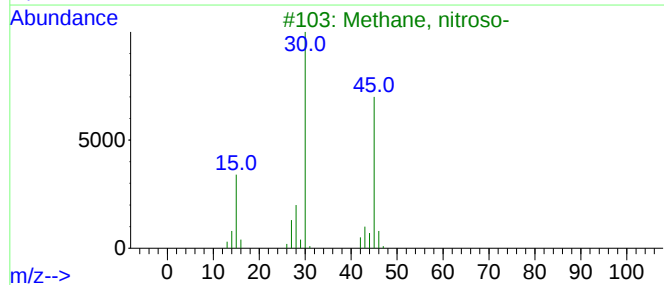
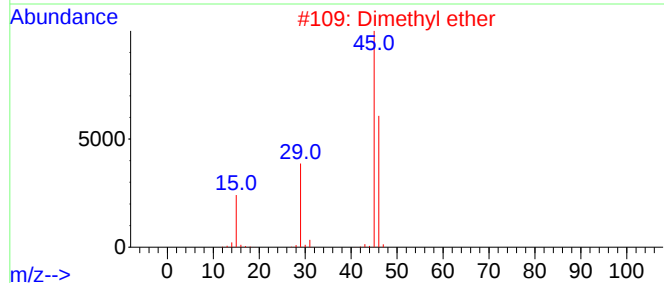
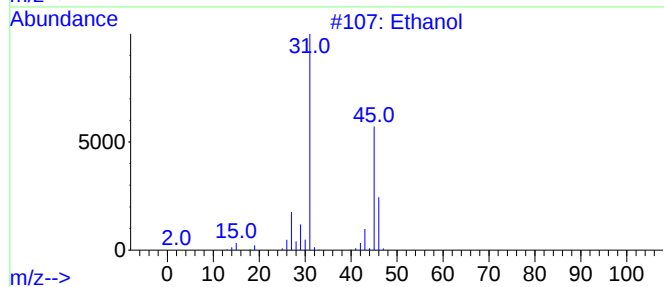
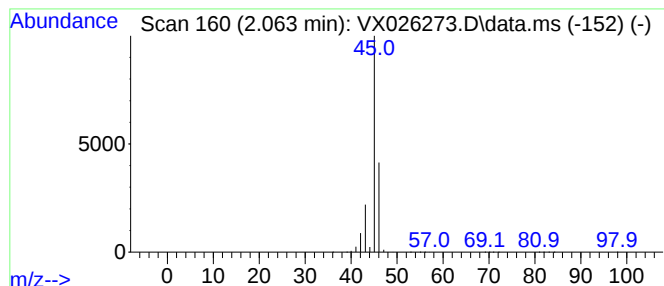
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.063	176.30 ug/l	1719580	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	64
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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ClientSampleId :
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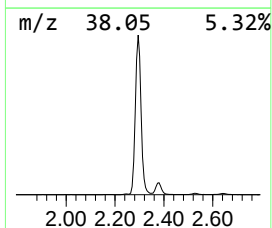
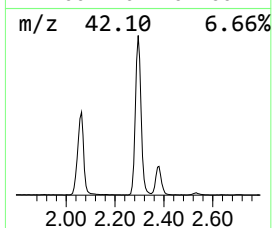
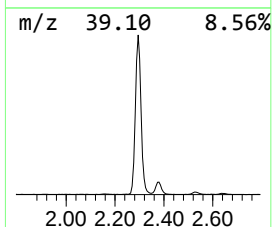
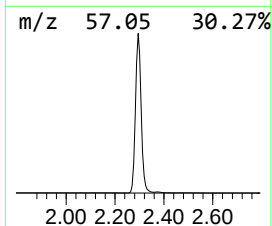
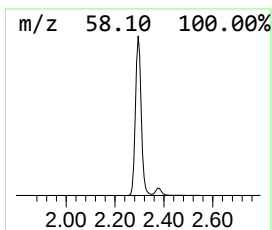
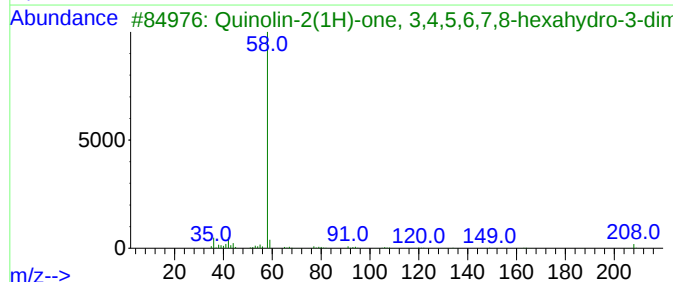
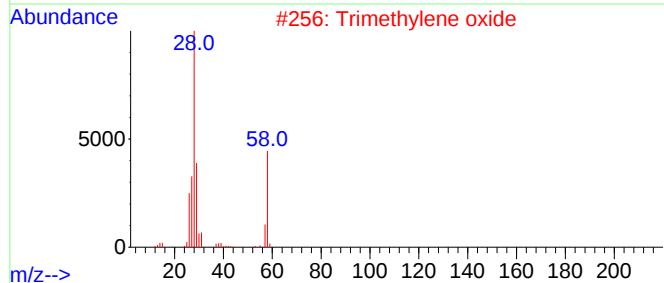
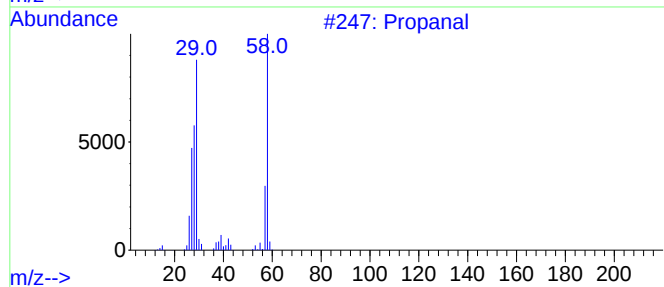
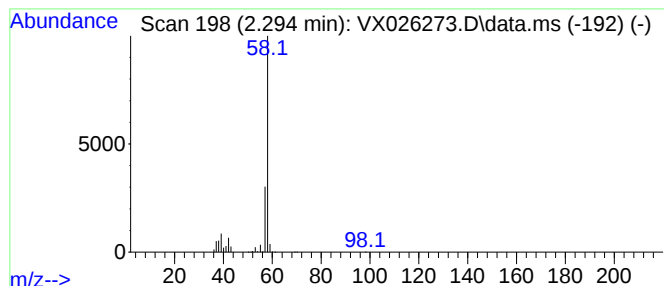
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 3 Propanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.294	410.63 ug/l	4005080	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal	58	C3H6O	000123-38-6	78
2			Trimethylene oxide	58	C3H6O	000503-30-0	56
3			Quinolin-2(1H)-one, 3,4,5,6,7,8-...	208	C12H20N2O	1000259-95-6	9
4			2-(Aminomethyl)-4-methylpentanoi...	187	C10H21NO2	1891211-54-3	9
5			Propylene oxide	58	C3H6O	000075-56-9	7



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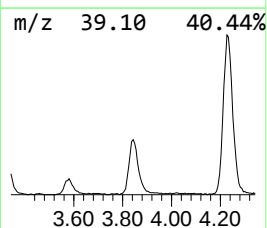
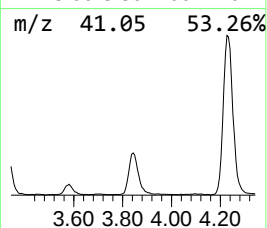
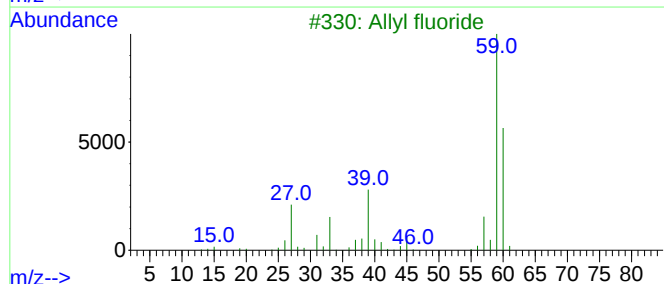
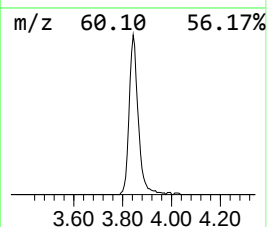
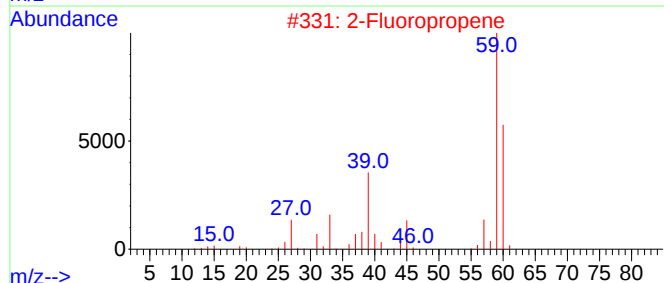
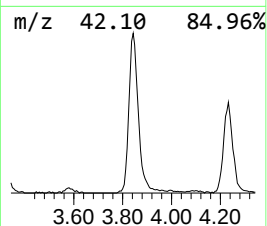
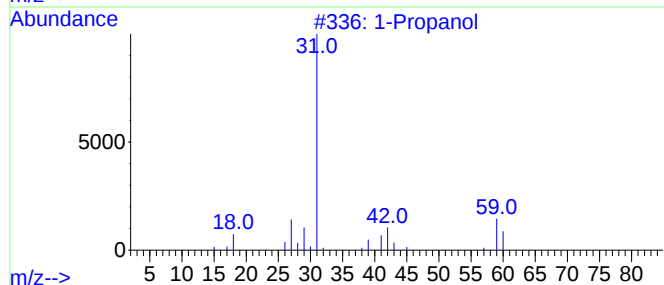
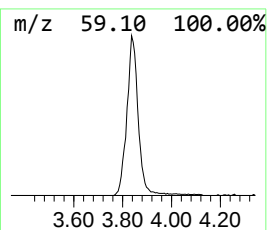
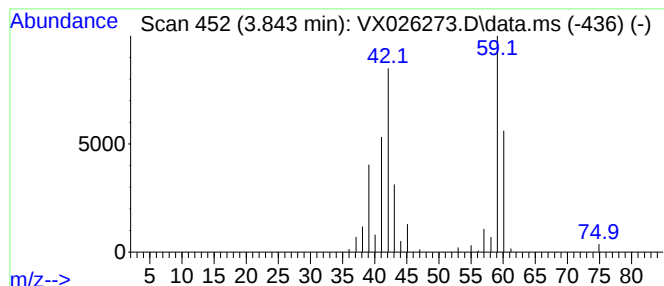
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.843	16.01 ug/l	156190	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	59
2			2-Fluoropropene	60	C3H5F	001184-60-7	52
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			3-Buten-1-ol	72	C4H8O	000627-27-0	32
5			Cyclopropane	42	C3H6	000075-19-4	25



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Instrument :
MSVOA_X
ClientSampleId :
20995

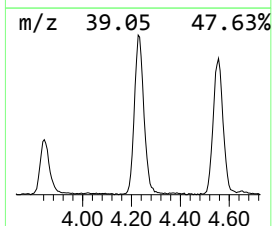
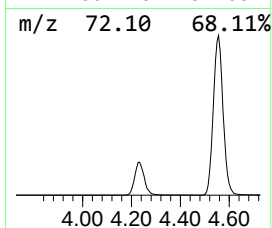
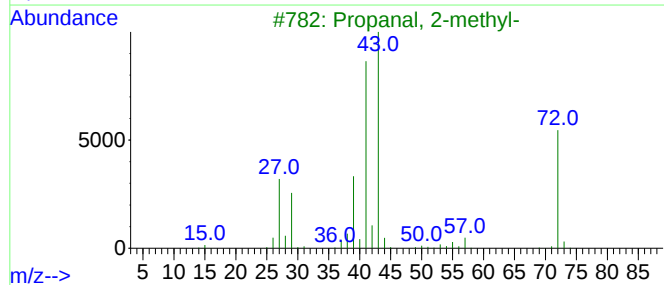
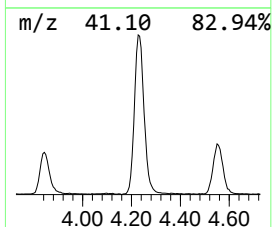
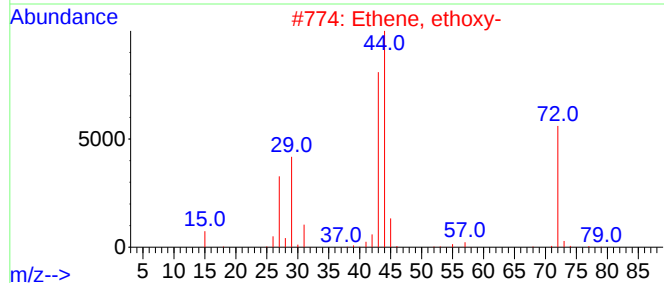
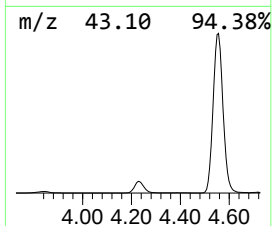
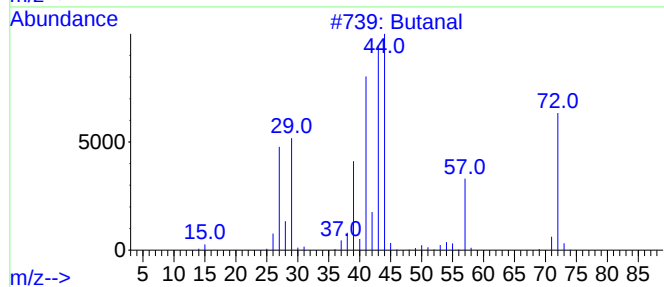
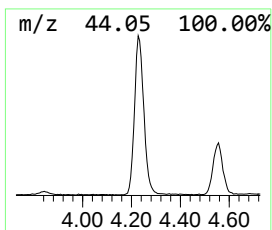
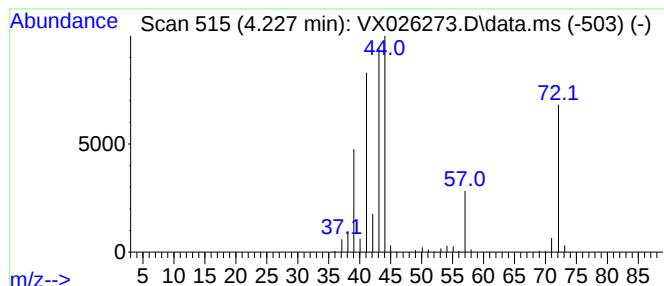
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Quant Title : SW846 8260

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

Peak Number 5 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.227	39.72 ug/l	387429	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	94
2			Ethene, ethoxy-	72	C4H8O	000109-92-2	49
3			Propanal, 2-methyl-	72	C4H8O	000078-84-2	43
4			2-Propen-1-ol, 2-methyl-, acetate	114	C6H10O2	000820-71-3	23
5			Isobutylene epoxide	72	C4H8O	000558-30-5	22



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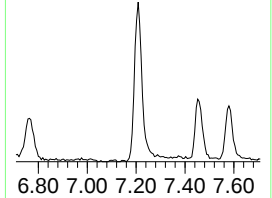
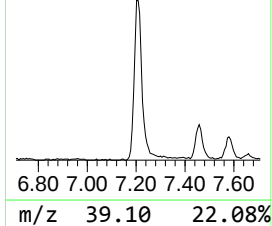
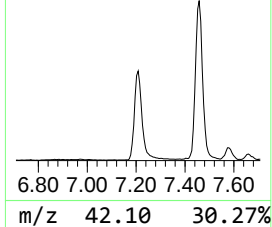
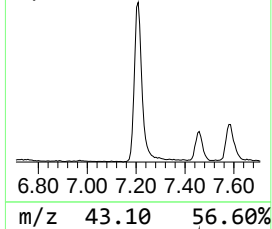
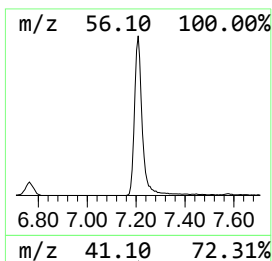
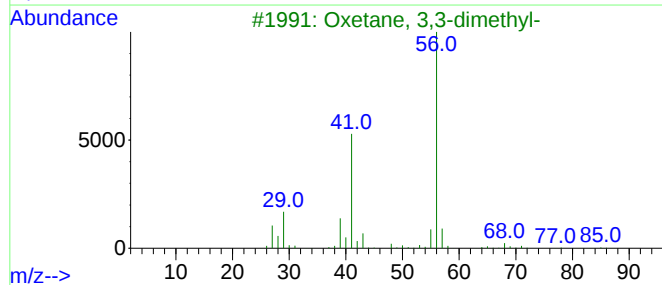
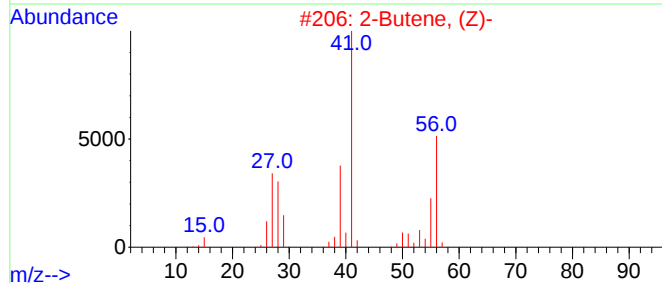
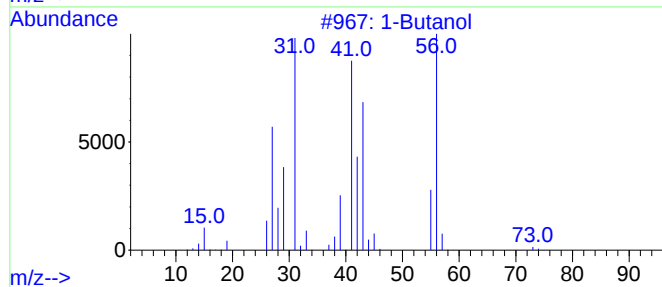
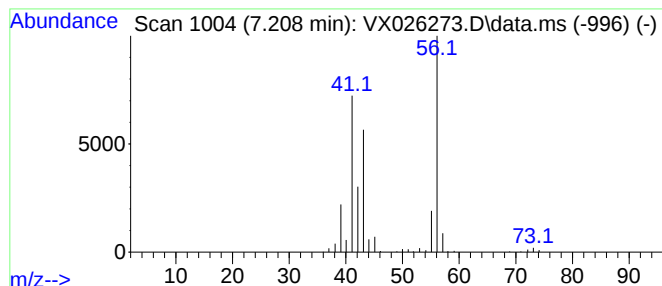
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 6 1-Butanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.208	19.11 ug/l	249248	1,4-Difluorobenzene	6.763

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol		74	C4H10O	000071-36-3	91
2	2-Butene, (Z)-		56	C4H8	000590-18-1	9
3	Oxetane, 3,3-dimethyl-		86	C5H10O	006921-35-3	9
4	Butane, 1-chloro-		92	C4H9Cl	000109-69-3	9
5	Propane, 2-cyclopropyl-		84	C6H12	003638-35-5	9



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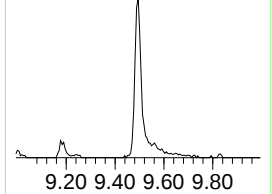
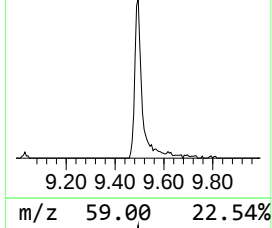
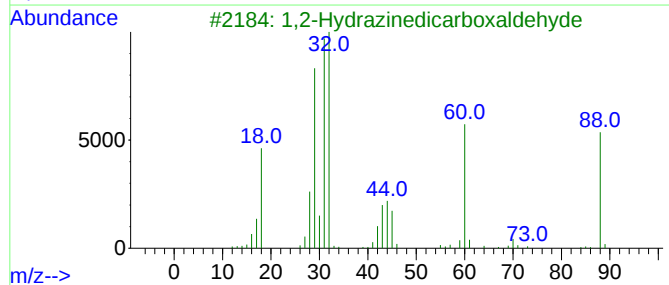
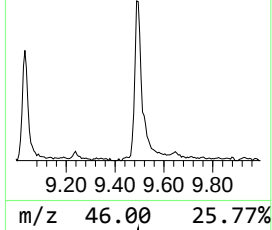
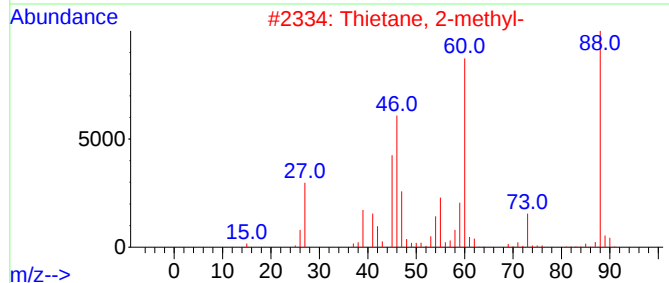
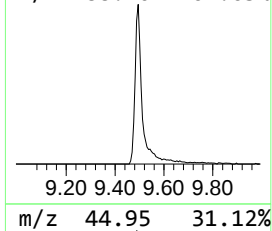
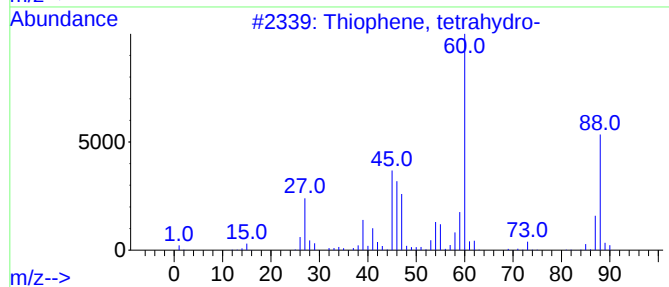
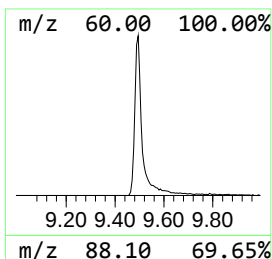
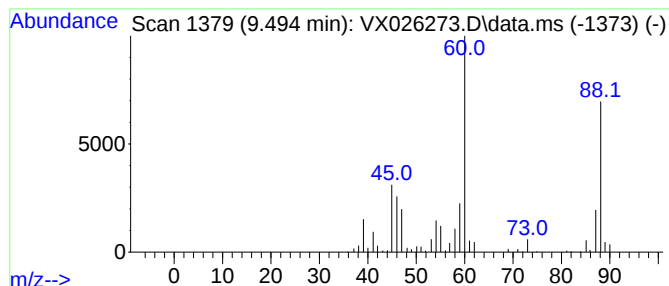
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Quant Title : SW846 8260

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

Peak Number 7 Thiophene, tetrahydro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.494	12.70 ug/l	193900	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2			Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3			1,2-Hydrazinedicarboxaldehyde	88	C2H4N2O2	000628-36-4	50
4			Ethylvinyl sulfide	88	C4H8S	000627-50-9	40
5			Ethanone, 1-(5-methylfur-2-yl)-,...	197	C8H11N3OS	090090-78-1	17



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\WX010422\
Data File : VX026273.D
Acq On : 04 Jan 2022 15:51
Operator : JC/MD
Sample : M5328-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20995

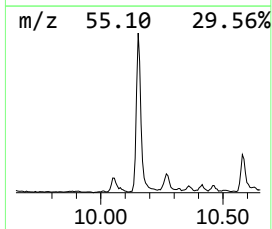
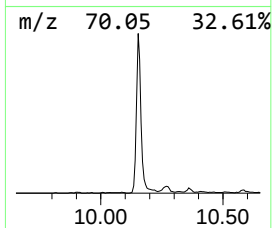
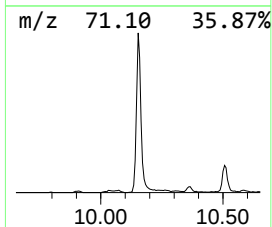
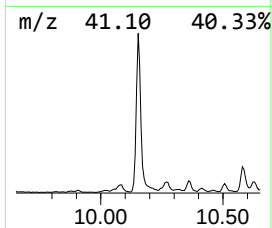
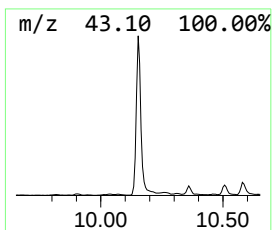
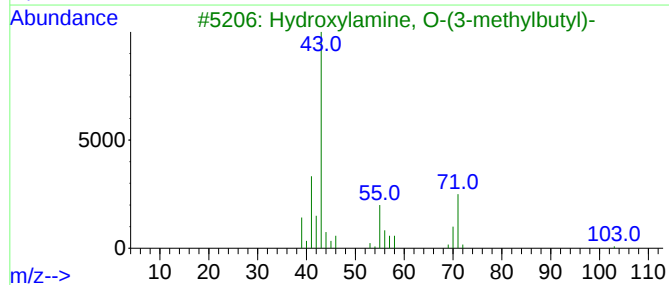
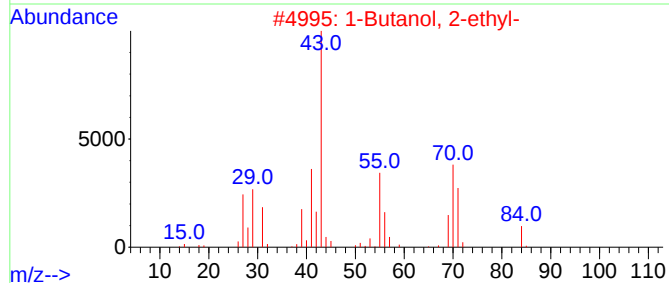
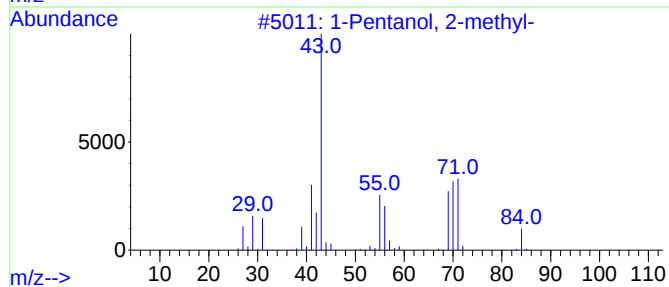
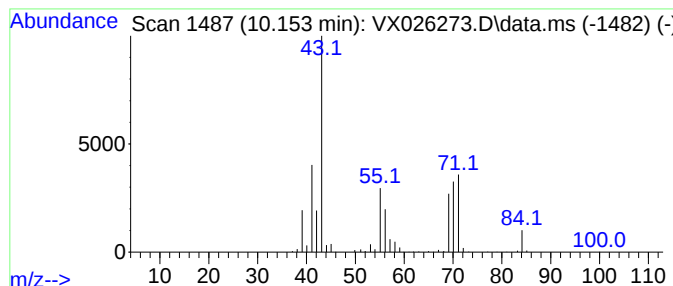
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Quant Title : SW846 8260

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

Peak Number 8 1-Pentanol, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.153	24.70 ug/l	377055	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	90
2			1-Butanol, 2-ethyl-	102	C6H14O	000097-95-0	83
3			Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	47
4			Pyrrolidine	71	C4H9N	000123-75-1	42
5			1-Fluorooctane	132	C8H17F	000463-11-6	42



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
Data File : VX026273.D
Acq On : 04 Jan 2022 15:51
Operator : JC/MD
Sample : M5328-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20995

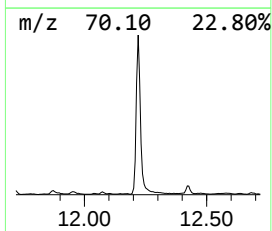
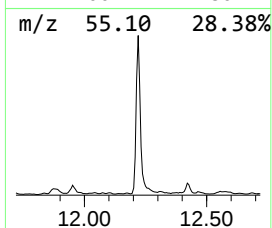
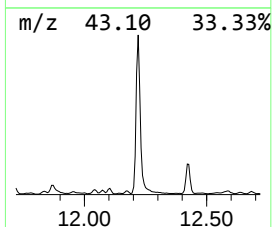
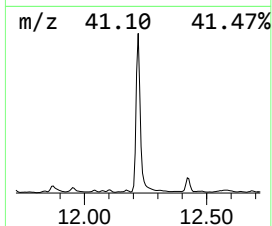
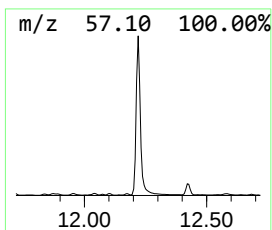
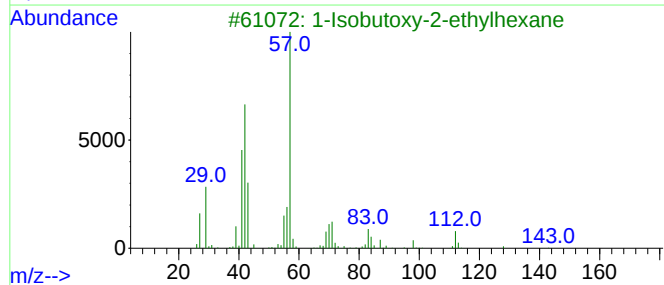
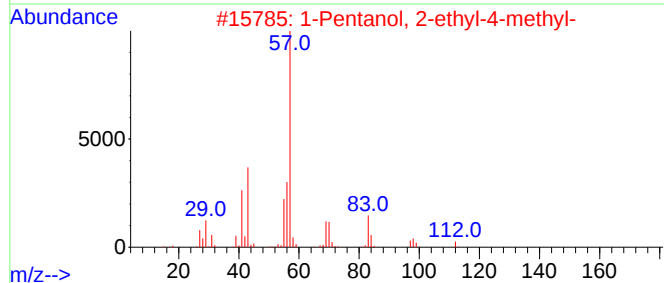
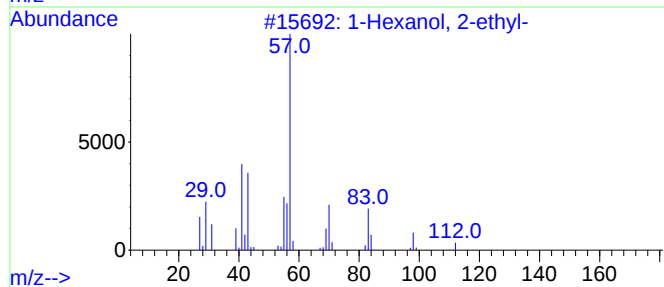
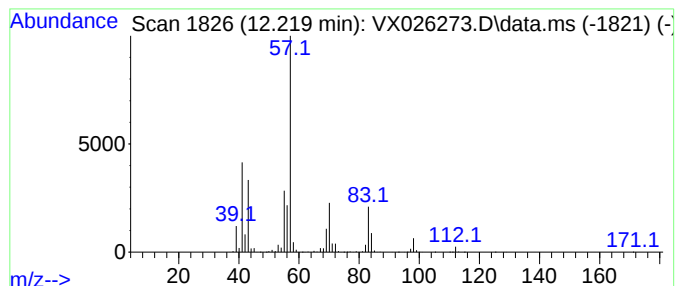
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Quant Title : SW846 8260

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.219	130.57 ug/l	1873230	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	47
5			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
Data File : VX026273.D
Acq On : 04 Jan 2022 15:51
Operator : JC/MD
Sample : M5328-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20995

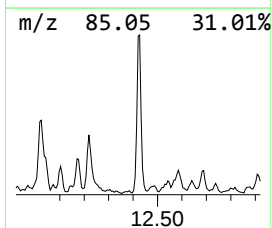
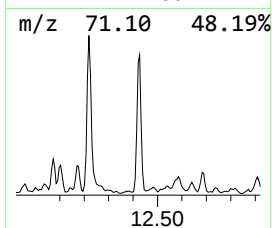
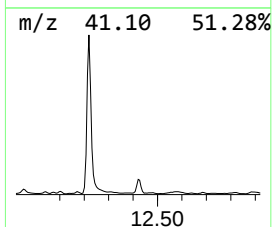
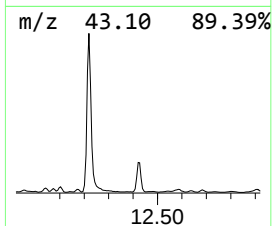
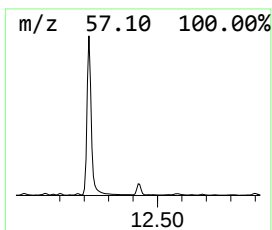
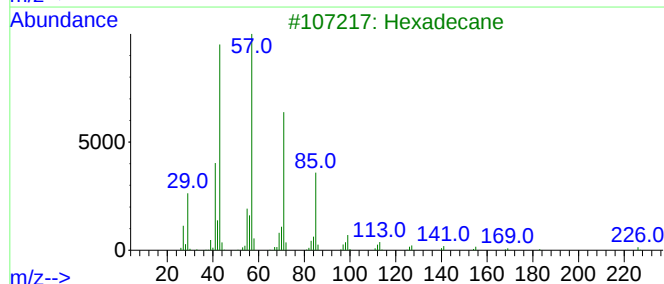
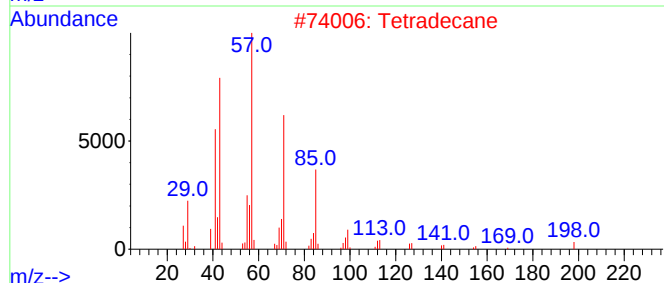
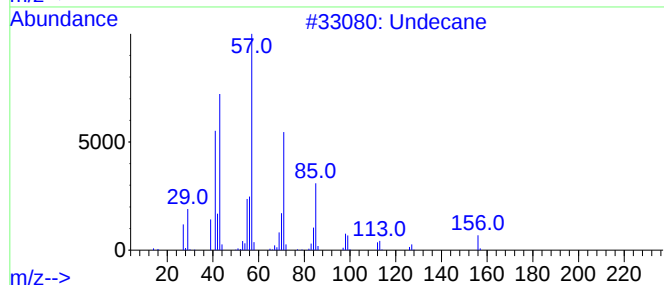
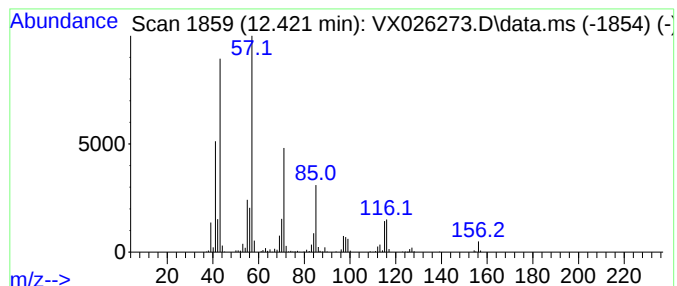
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.M
Quant Title : SW846 8260

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

Peak Number 10 Undecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.421	13.71 ug/l	196643	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Undecane	156	C11H24	001120-21-4	96
2			Tetradecane	198	C14H30	000629-59-4	72
3			Hexadecane	226	C16H34	000544-76-3	58
4			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53
5			Dodecane, 2-methyl-	184	C13H28	001560-97-0	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX010422\
Data File : VX026273.D
Acq On : 04 Jan 2022 15:51
Operator : JC/MD
Sample : M5328-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
20995

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X123021W.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
Ethanol	2.063	176.3	ug/l	1719580	1	5.556	487681	50.0
Propanal	2.294	410.6	ug/l	4005080	1	5.556	487681	50.0
1-Propanol	3.843	16.0	ug/l	156190	1	5.556	487681	50.0
Butanal	4.227	39.7	ug/l	387429	1	5.556	487681	50.0
1-Butanol	7.208	19.1	ug/l	249248	2	6.763	652041	50.0
Thiophene, tetr...	9.494	12.7	ug/l	193900	3	10.055	763423	50.0
1-Pentanol, 2-m...	10.153	24.7	ug/l	377055	3	10.055	763423	50.0
1-Hexanol, 2-et...	12.219	130.6	ug/l	1873230	4	12.024	717351	50.0
Undecane	12.421	13.7	ug/l	196643	4	12.024	717351	50.0