

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX053119\
 Data File : VX009979.D
 Acq On : 31 May 2019 12:24
 Operator : JC/SP
 Sample : K2964-02
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-2

Integration Parameters: RTEINT.P

Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
 Title : SW846 8260

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.276	16	20	24	rBV	232697	322433	1.22%	0.337%
2	1.489	51	55	66	rVB	541037	668810	2.54%	0.699%
3	2.172	151	167	170	rBV	6545997	17557580	66.58%	18.347%
4	2.452	205	213	228	rBV	7594867	13109086	49.71%	13.699%
5	2.629	233	242	259	rVV	4180502	7637197	28.96%	7.981%
6	2.776	260	266	276	rVB	394495	694633	2.63%	0.726%
7	3.989	450	465	481	rBV	1142775	3310520	12.55%	3.459%
8	4.836	593	604	621	rVB	224116	652062	2.47%	0.681%
9	5.501	702	713	724	rVB	102144	287949	1.09%	0.301%
10	5.659	729	739	761	rVB	180897	522400	1.98%	0.546%
11	6.062	795	805	817	rBV	128199	334470	1.27%	0.350%
12	6.226	822	832	845	rBV	155485	411800	1.56%	0.430%
13	6.860	926	936	951	rBV	298554	717729	2.72%	0.750%
14	7.305	1001	1009	1028	rVB	1019490	2053256	7.79%	2.146%
15	8.714	1234	1240	1246	rBV	624301	964606	3.66%	1.008%
16	9.293	1330	1335	1340	rBV	333895	493624	1.87%	0.516%
17	9.439	1353	1359	1364	rBV	355304	506040	1.92%	0.529%
18	10.110	1464	1469	1481	rVB	603283	833358	3.16%	0.871%
19	10.634	1550	1555	1559	rBV	690592	850197	3.22%	0.888%
20	11.134	1631	1637	1647	rBV	530930	718595	2.72%	0.751%
21	11.804	1743	1747	1757	rVB3	276787	424857	1.61%	0.444%
22	11.945	1765	1770	1773	rBV2	177297	268753	1.02%	0.281%
23	12.073	1785	1791	1797	rVB2	612071	944908	3.58%	0.987%
24	12.152	1797	1804	1810	rBV4	215947	488470	1.85%	0.510%
25	12.268	1819	1823	1829	rBV	1355062	1605053	6.09%	1.677%
26	12.475	1853	1857	1861	rVB	313811	347853	1.32%	0.363%
27	12.646	1879	1885	1898	rVB	21114581	26372236	100.00%	27.558%
28	13.018	1941	1946	1953	rVB3	228610	419373	1.59%	0.438%
29	13.201	1971	1976	1984	rVB2	566741	827577	3.14%	0.865%
30	13.316	1990	1995	1997	rBV	247622	304018	1.15%	0.318%
31	13.347	1997	2000	2004	rVB2	210498	290359	1.10%	0.303%
32	13.475	2017	2021	2031	rBV	1381878	1762236	6.68%	1.842%
33	13.640	2043	2048	2058	rVB3	347018	742987	2.82%	0.776%
34	14.091	2118	2122	2126	rVB	266046	278242	1.06%	0.291%

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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

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35	14.249	2144	2148	2164	rBV	3923751	5318349	20.17%	5.558%
36	15.188	2297	2302	2309	rBV	950882	1451083	5.50%	1.516%
37	15.279	2313	2317	2324	rVB	527242	822939	3.12%	0.860%
38	16.176	2457	2464	2480	rBV	198125	380042	1.44%	0.397%

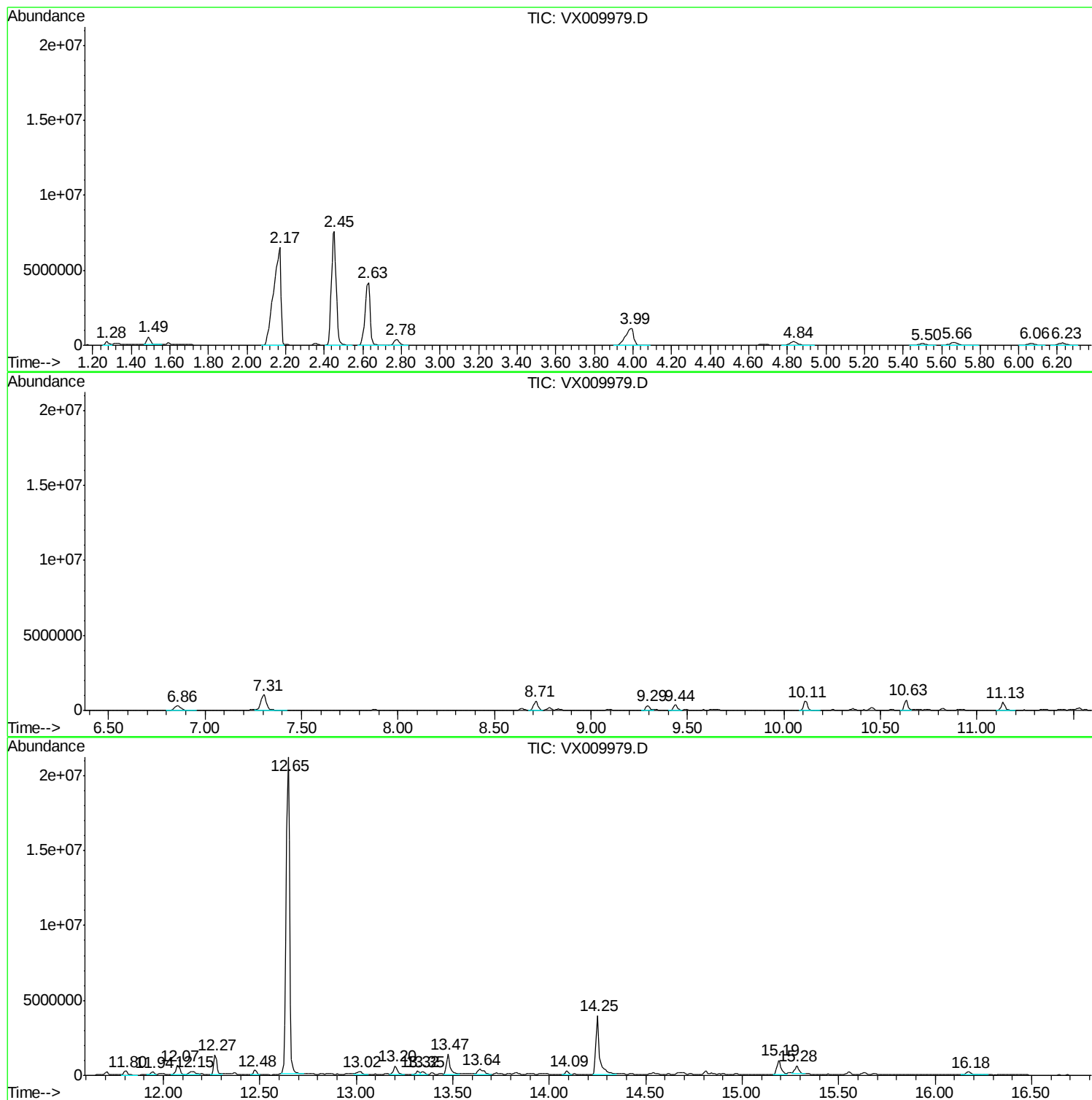
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Quant Title : SW846 8260

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



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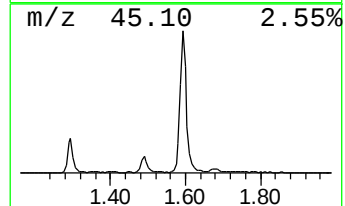
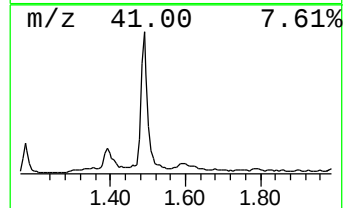
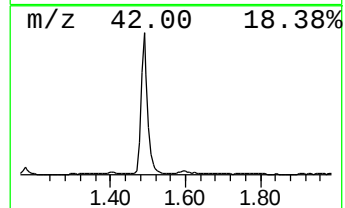
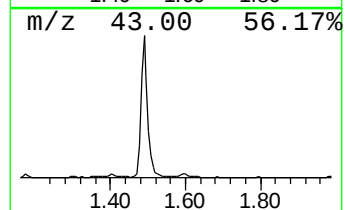
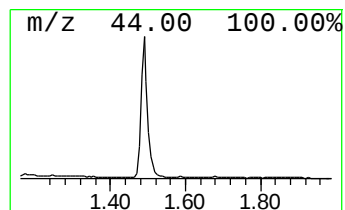
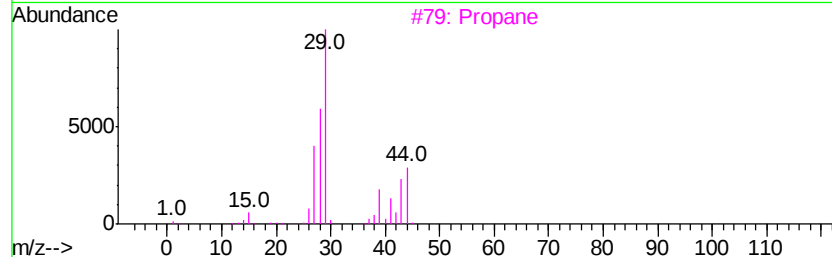
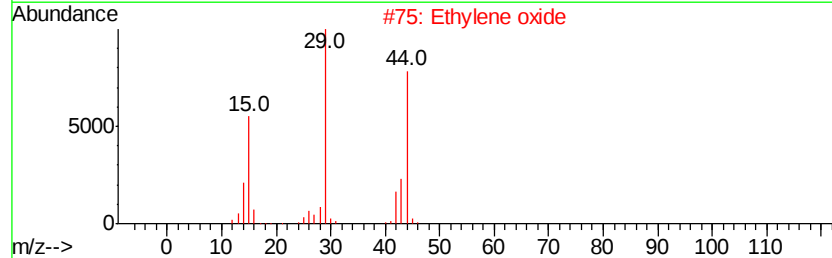
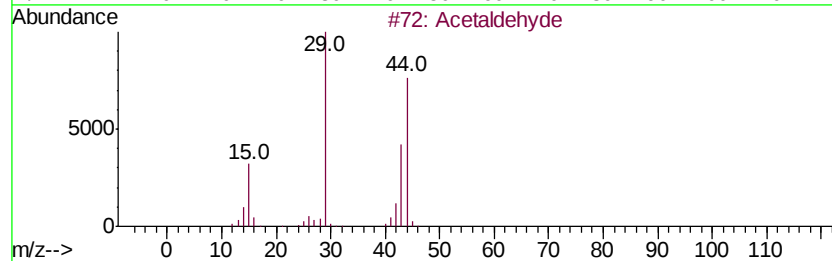
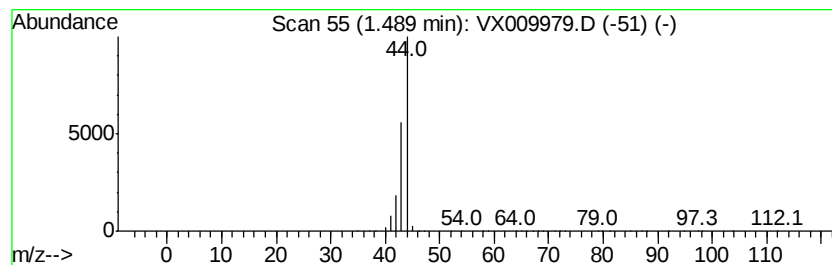
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 1 Acetaldehyde Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	64.01 ug/l	668810	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		Acetic acid, [(aminocarbonyl)ami...	132	C3H4N2O4	000585-05-7	4
5		2-Propanamine	59	C3H9N	000075-31-0	4



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ClientSampleId :
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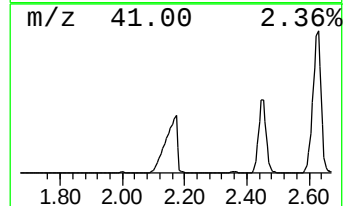
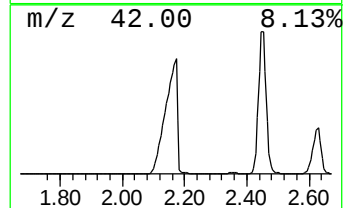
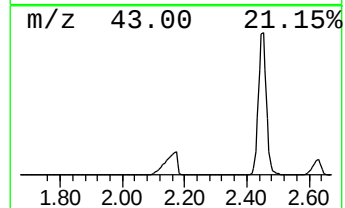
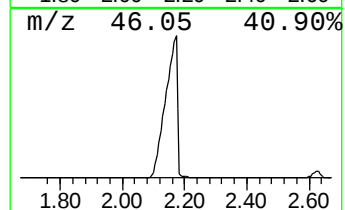
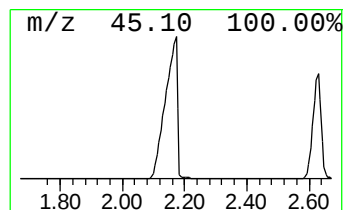
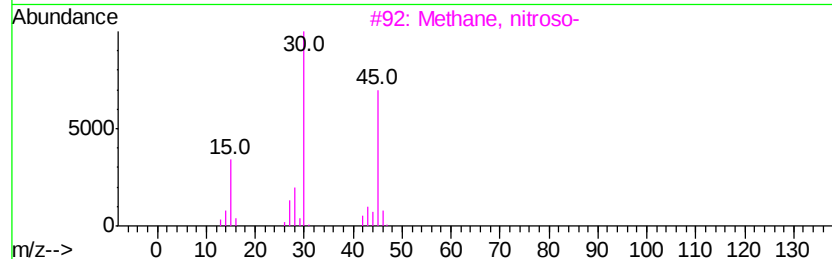
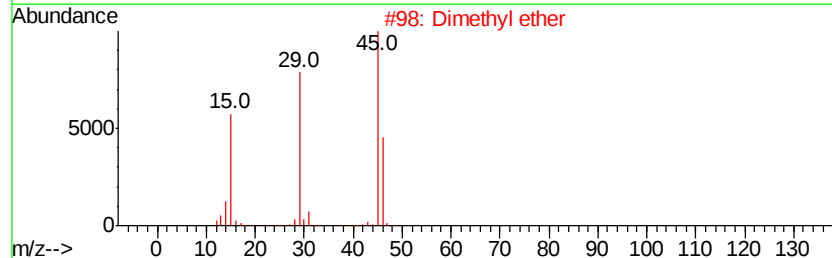
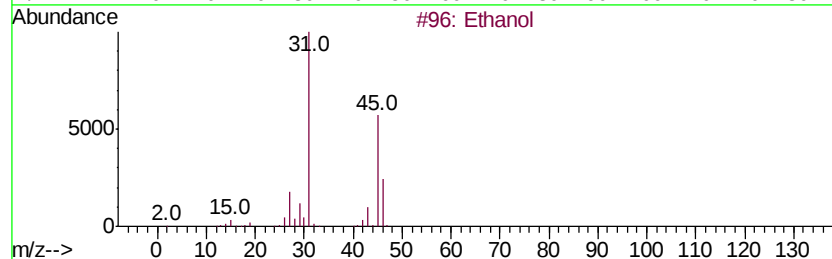
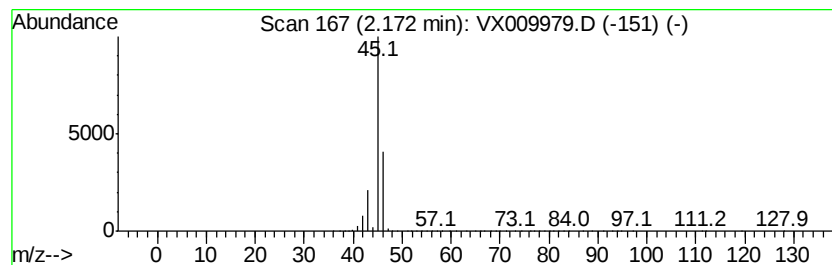
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	1680.47 ug/l	17557600	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	83
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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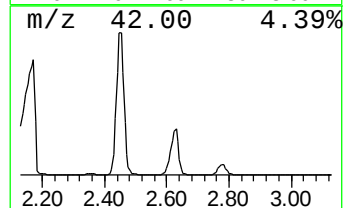
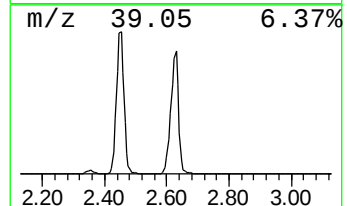
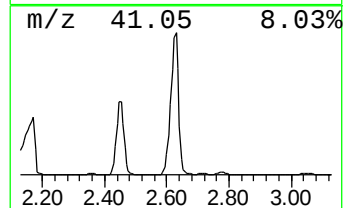
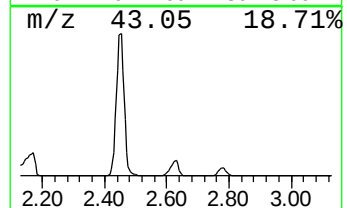
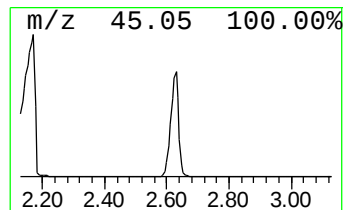
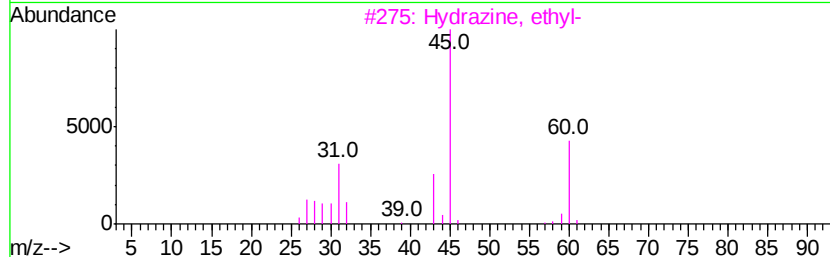
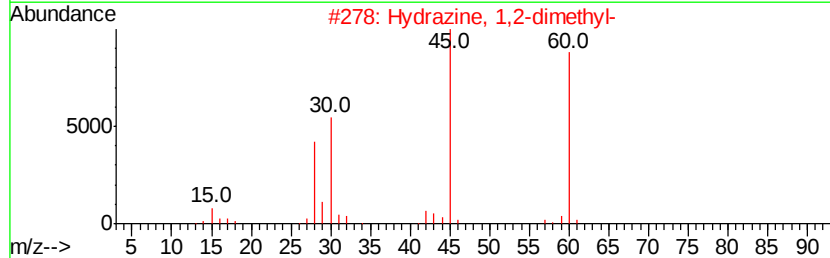
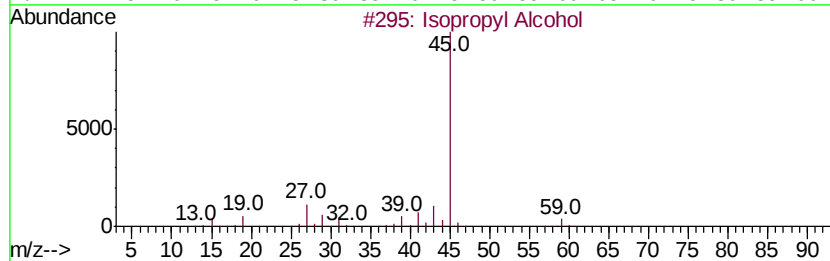
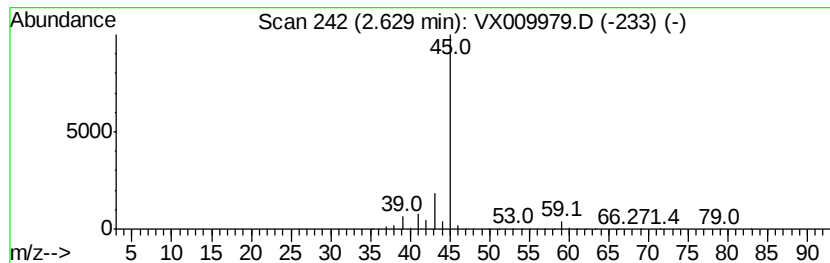
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.63	730.97 ug/l	7637200	Pentafluorobenzene	5.67

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isopropyl Alcohol	60	C3H8O	000067-63-0	78
2		Hvdrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		Hvdrazine, ethyl-	60	C2H8N2	000624-80-6	9
4		Formamide	45	CH3NO	000075-12-7	5
5		4-Penten-2-ol	86	C5H10O	000625-31-0	4



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Instrument :
MSVOA_X
ClientSampled :
COMP-2

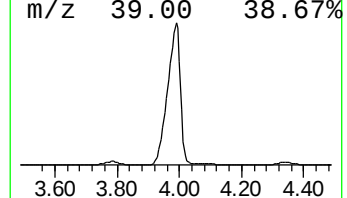
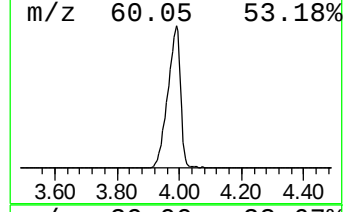
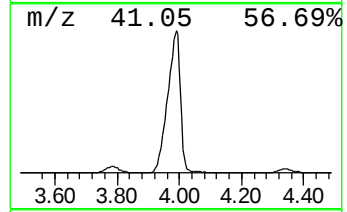
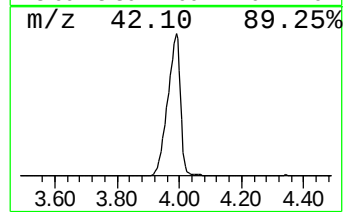
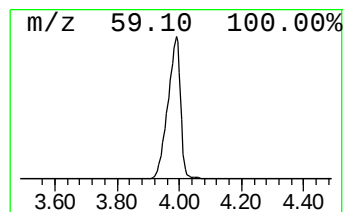
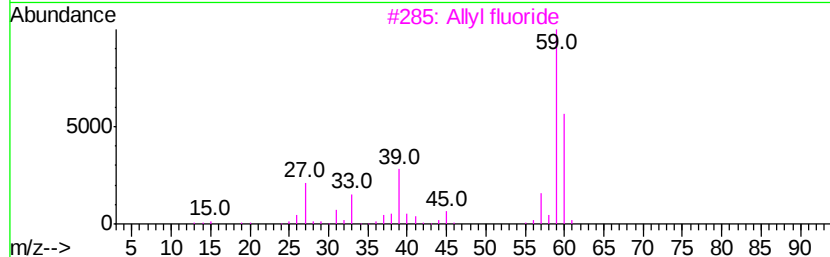
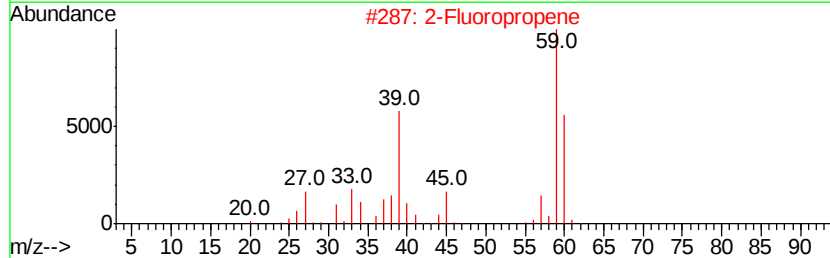
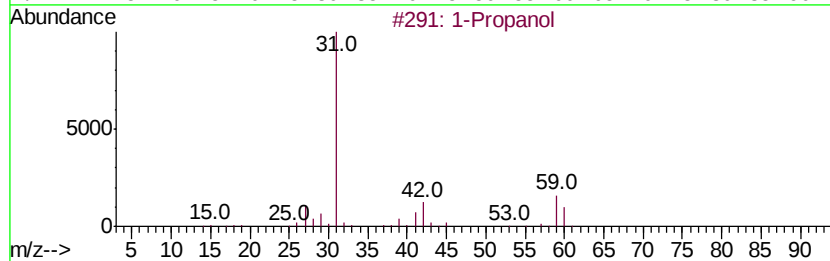
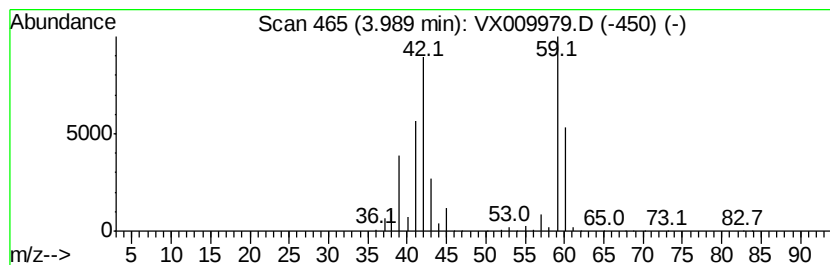
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.99	316.86 ug/l	3310520	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	64
2		2-Fluoropropene	60	C3H5F	001184-60-7	50
3		Allyl fluoride	60	C3H5F	000818-92-8	32
4		Propene	42	C3H6	000115-07-1	9
5		Cyclopropane	42	C3H6	000075-19-4	9



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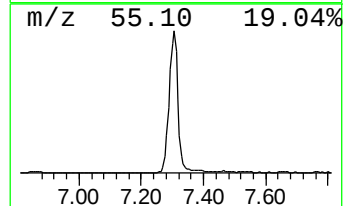
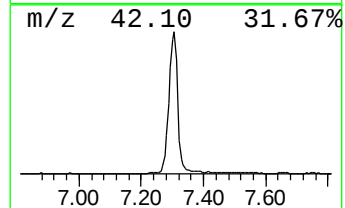
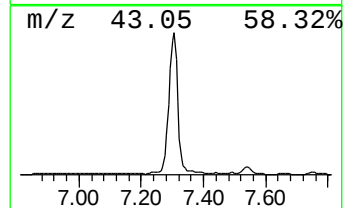
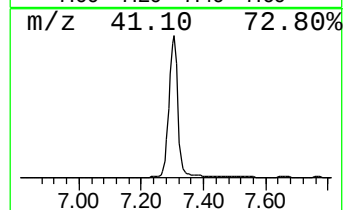
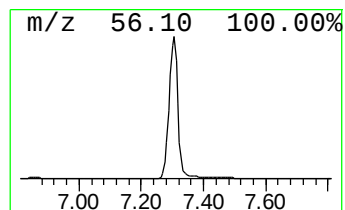
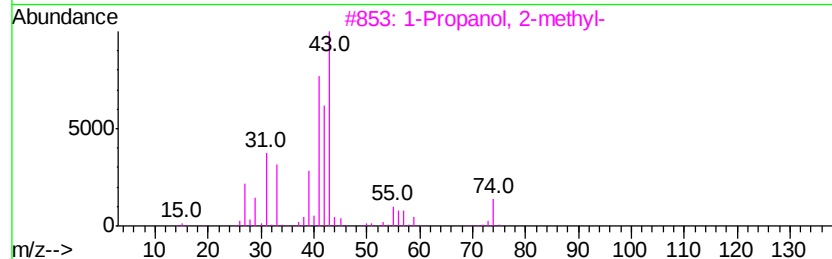
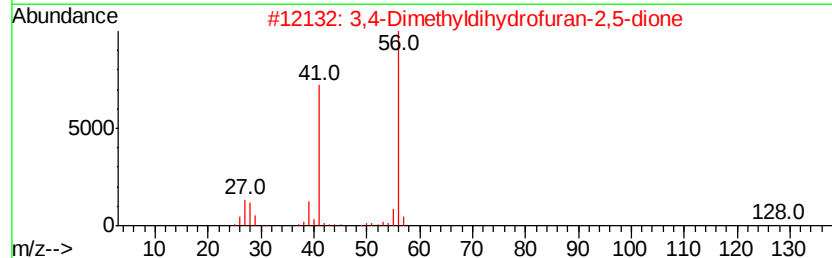
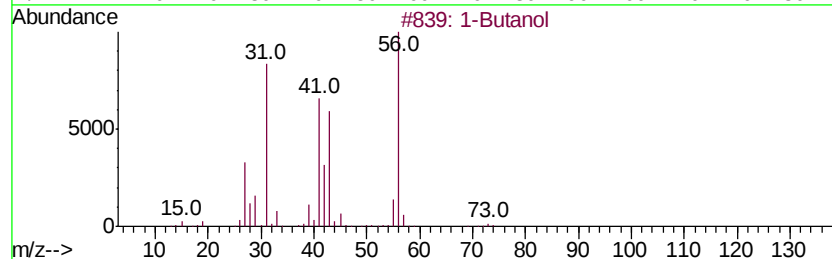
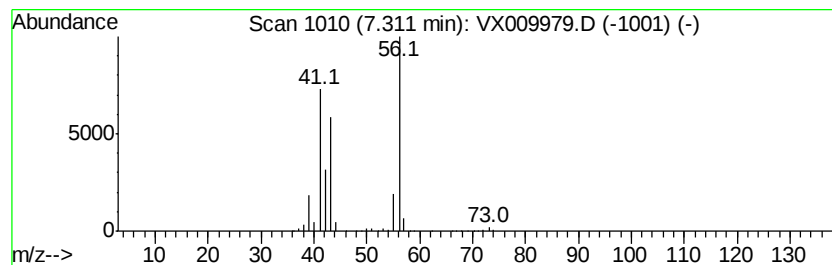
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.31	143.04 ug/l	2053260	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Butanol	74	C4H10O	000071-36-3	90
2		3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	36
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	10
4		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	9
5		Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

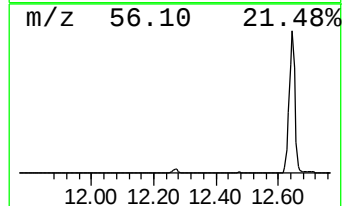
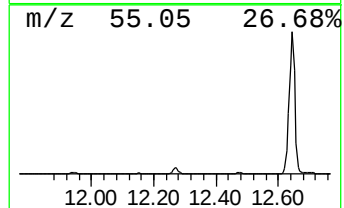
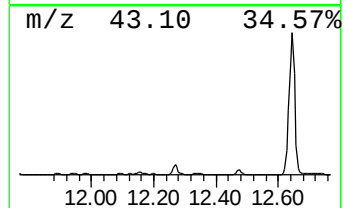
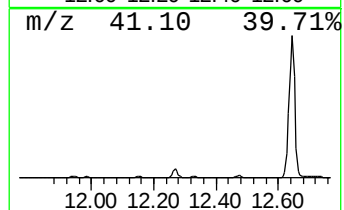
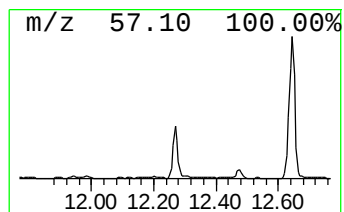
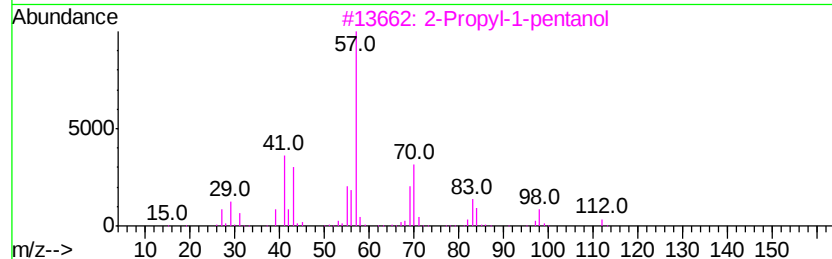
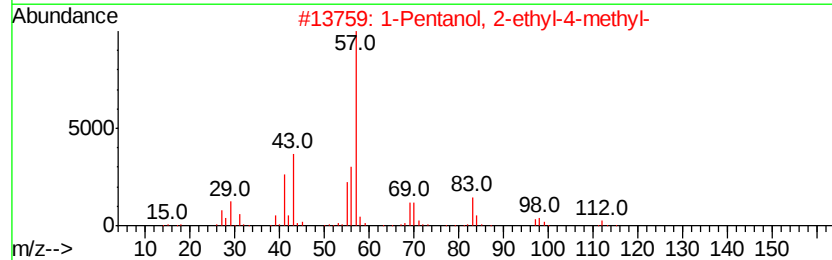
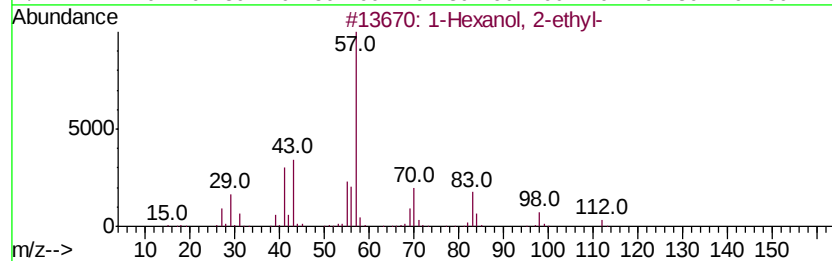
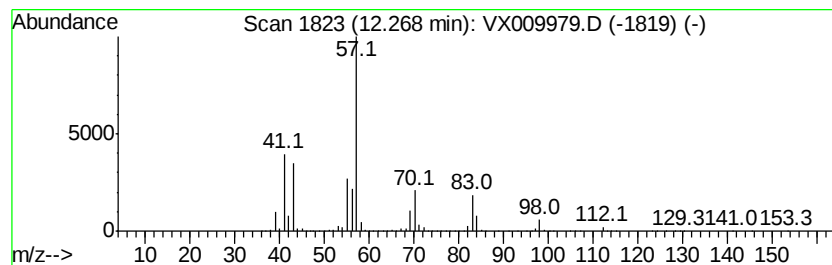
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Quant Title : SW846 8260

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

Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	84.93 ug/l	1605050	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		Octane, 2,3-dimethyl-	142	C10H22	007146-60-3	45
5		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

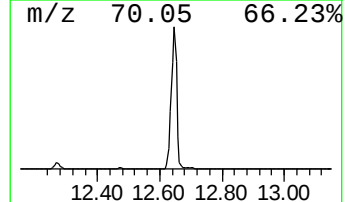
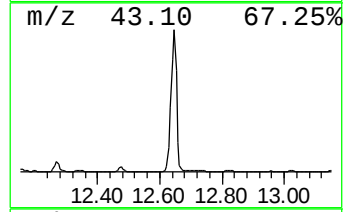
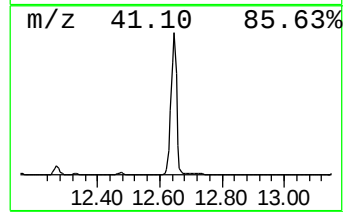
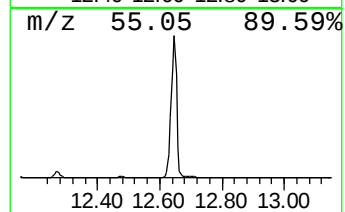
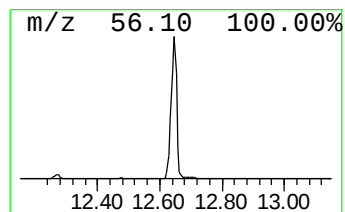
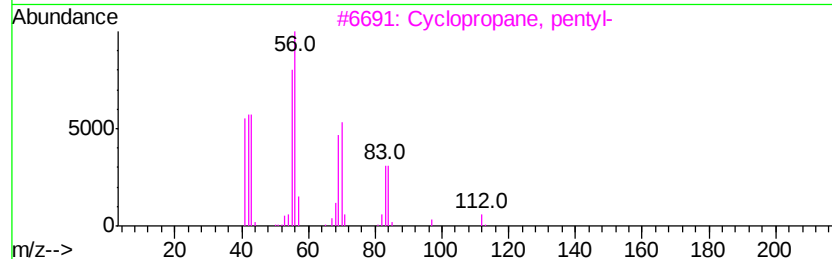
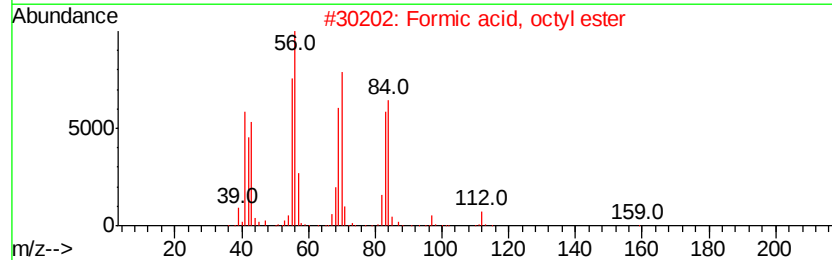
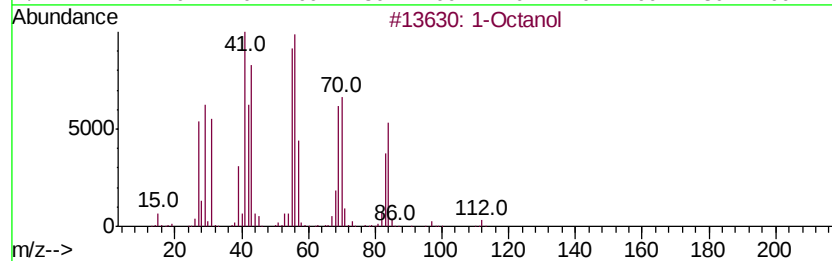
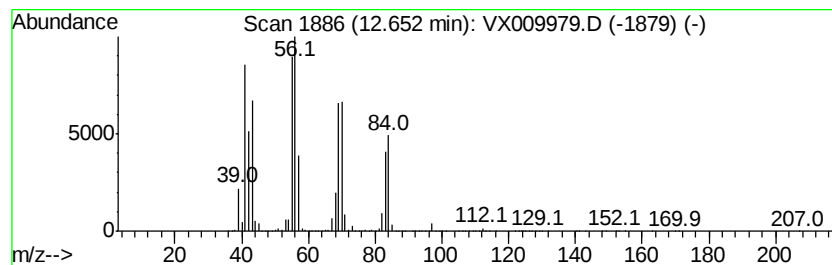
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Quant Title : SW846 8260

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

Peak Number 7 1-Octanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.65	1395.49 ug/l	26372200	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Octanol		130	C8H18O	000111-87-5	91
2	Formic acid, octyl ester		158	C9H18O2	000112-32-3	90
3	Cyclopropane, pentyl-		112	C8H16	002511-91-3	78
4	Cyclooctane		112	C8H16	000292-64-8	78
5	Cyclobutane, 1,2-diethyl-, cis-		112	C8H16	061141-50-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

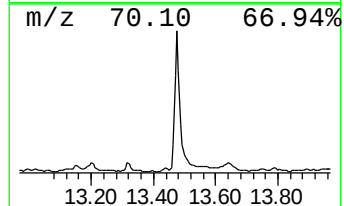
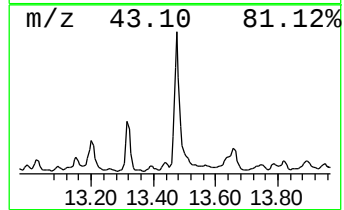
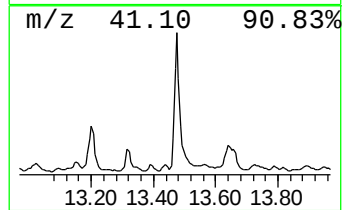
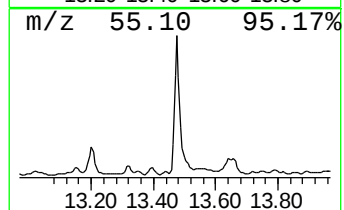
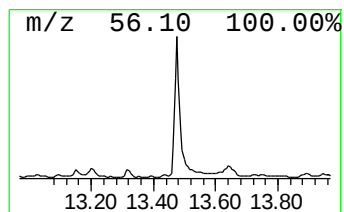
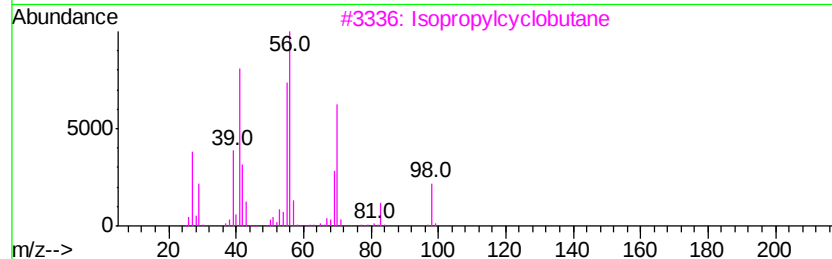
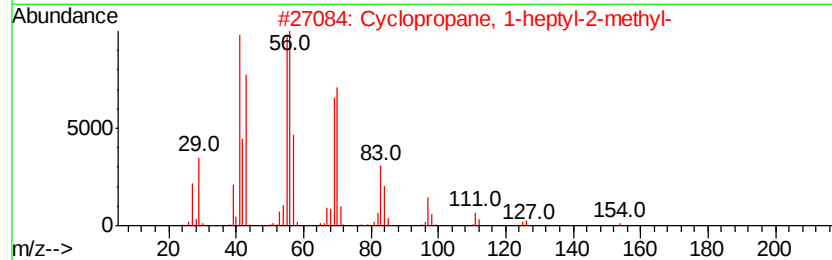
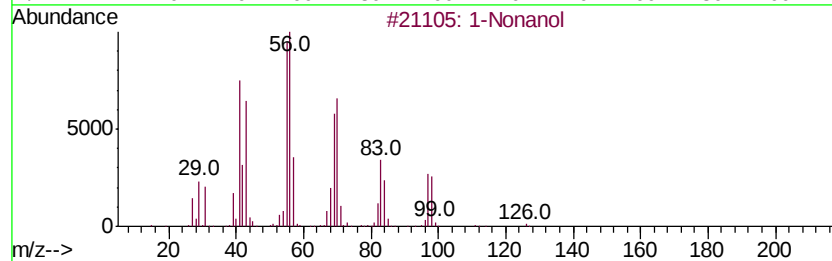
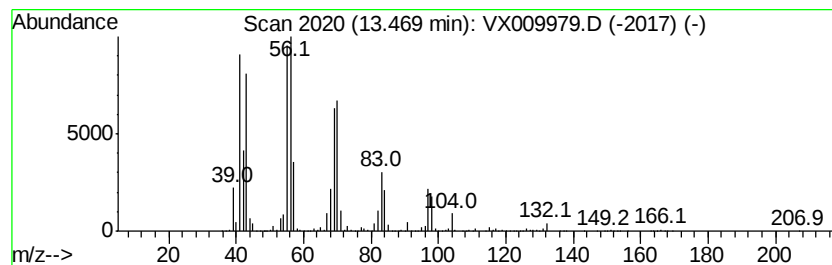
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Quant Title : SW846 8260

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

Peak Number 8 1-Nonanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.47	93.25 ug/l	1762240	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Nonanol	144	C9H20O	000143-08-8	87
2		Cyclopropane, 1-heptyl-2-methyl-	154	C11H22	074663-91-5	64
3		Isopropylcyclobutane	98	C7H14	000872-56-0	62
4		1-Heptene	98	C7H14	000592-76-7	58
5		Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	58



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

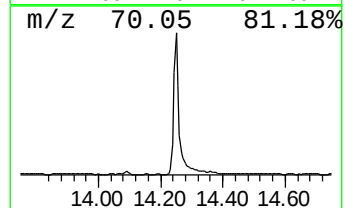
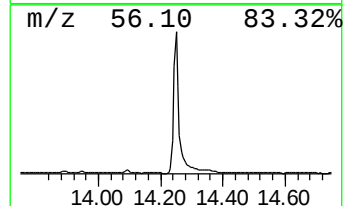
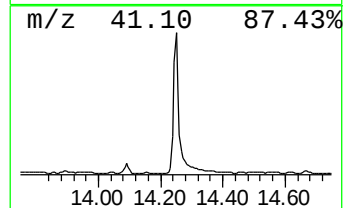
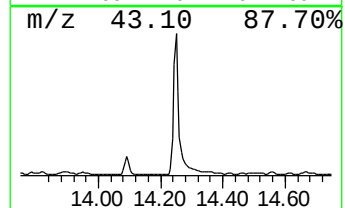
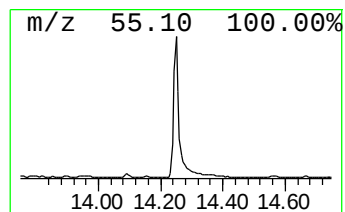
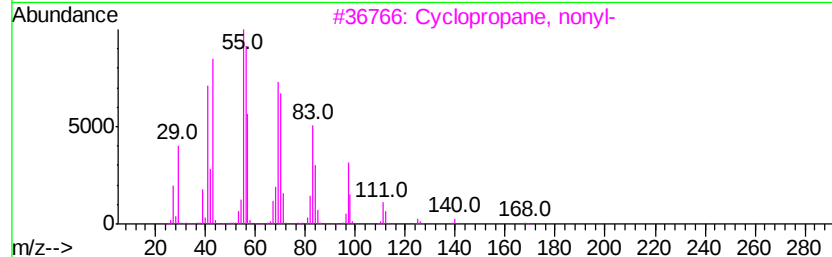
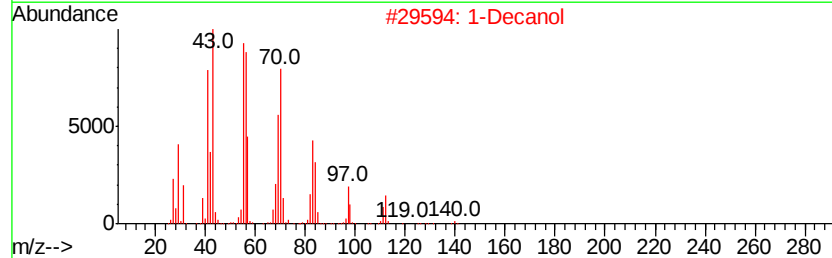
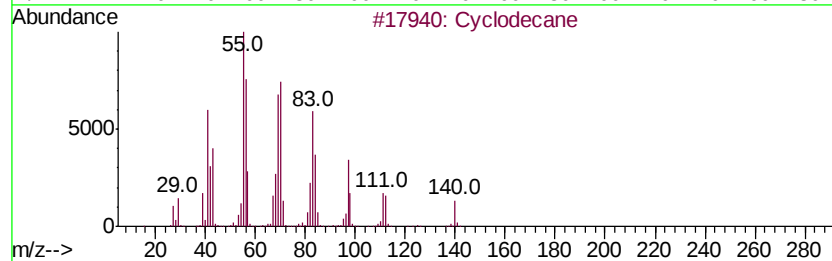
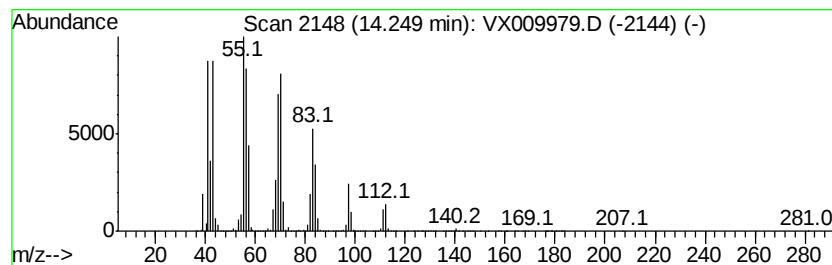
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 9 Cyclodecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.25	281.42 ug/l	5318350	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclodecane	140	C10H20	000293-96-9	94
2	1-Decanol	158	C10H22O	000112-30-1	91
3	Cyclopropane, nonyl-	168	C12H24	074663-85-7	90
4	Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	90
5	Cyclooctane	112	C8H16	000292-64-8	87



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

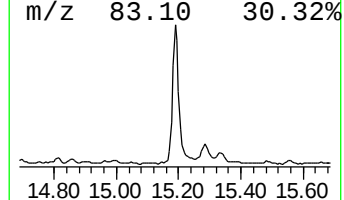
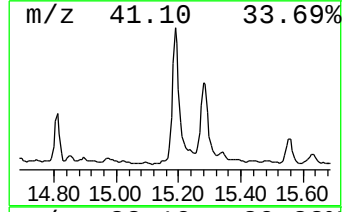
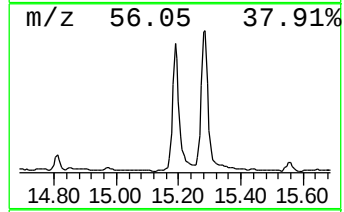
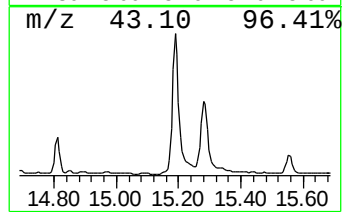
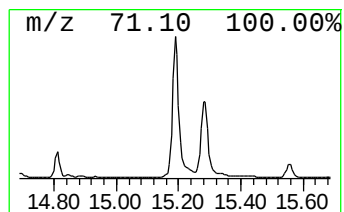
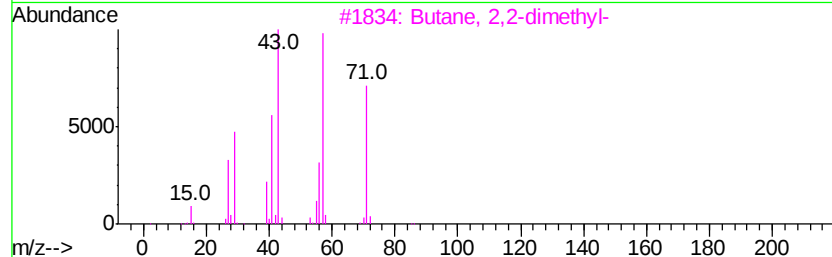
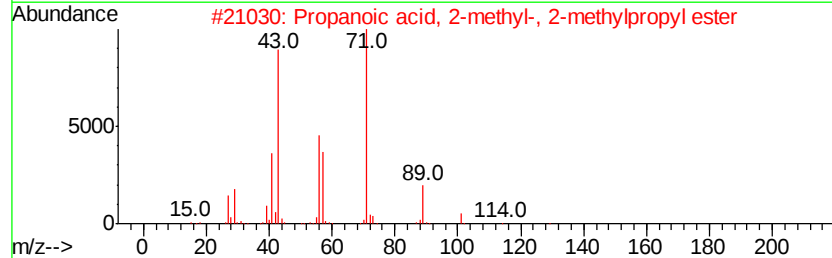
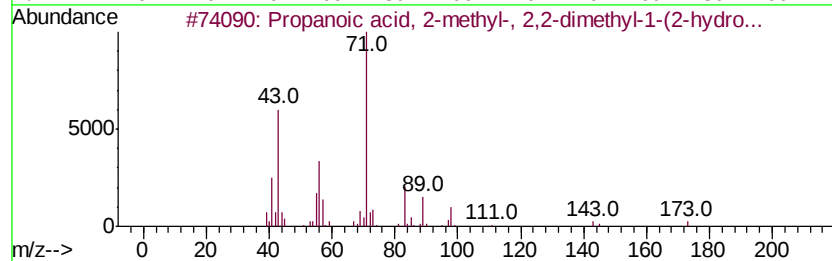
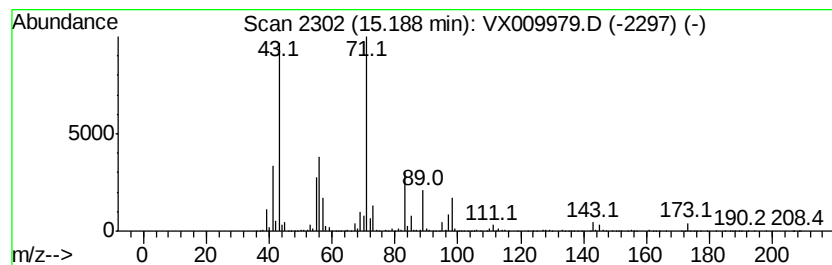
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 10 Propanoic acid, 2-methyl-, ... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.19	76.78 ug/l	1451080	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 2,2-d...	216	C12H24O3	074367-33-2	80
2		Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	50
3		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	43
4		Propanoic acid, 2-methyl-, 3-hyd...	216	C12H24O3	074367-34-3	43
5		1-Hexene, 3,4,5-trimethyl-	126	C9H18	056728-10-0	43



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX053119\
Data File : VX009979.D
Acq On : 31 May 2019 12:24
Operator : JC/SP
Sample : K2964-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-2

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.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	1.49	64.0	ug/l	668810	1	5.67	522400	50.0
Ethanol	2.17	1680.5	ug/l	17557600	1	5.67	522400	50.0
Isopropyl Alcohol	2.63	731.0	ug/l	7637200	1	5.67	522400	50.0
1-Propanol	3.99	316.9	ug/l	3310520	1	5.67	522400	50.0
1-Butanol	7.31	143.0	ug/l	2053260	2	6.86	717729	50.0
1-Hexanol, 2-ethyl-	12.27	84.9	ug/l	1605050	4	12.08	944908	50.0
1-Octanol	12.65	1395.5	ug/l	26372200	4	12.08	944908	50.0
1-Nonanol	13.47	93.3	ug/l	1762240	4	12.08	944908	50.0
Cyclodecane	14.25	281.4	ug/l	5318350	4	12.08	944908	50.0
Propanoic acid, 2...	15.19	76.8	ug/l	1451080	4	12.08	944908	50.0