

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX053119\
 Data File : VX009986.D
 Acq On : 31 May 2019 15:37
 Operator : JC/SP
 Sample : K2964-03
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 COMP-3

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\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	1.459	48	50	106	rVB	33239882	76009851	100.00%	72.290%
2	8.713	1233	1240	1246	rBV	678392	1046338	1.38%	0.995%
3	8.781	1246	1251	1257	rVV	1016152	1590824	2.09%	1.513%
4	10.110	1462	1469	1480	rVB	633164	880352	1.16%	0.837%
5	10.366	1504	1511	1525	rVB2	1217083	1647909	2.17%	1.567%
6	11.134	1632	1637	1642	rBV	617509	793112	1.04%	0.754%
7	11.737	1731	1736	1741	rBV	1072202	1255312	1.65%	1.194%
8	11.920	1762	1766	1774	rVB	597880	799841	1.05%	0.761%
9	12.073	1788	1791	1799	rVB	619600	811150	1.07%	0.771%
10	12.268	1815	1823	1833	rBV	4524537	5697196	7.50%	5.418%
11	13.536	2025	2031	2034	rBV	2780821	3422023	4.50%	3.255%
12	13.646	2043	2049	2057	rBV	8835042	11192041	14.72%	10.644%

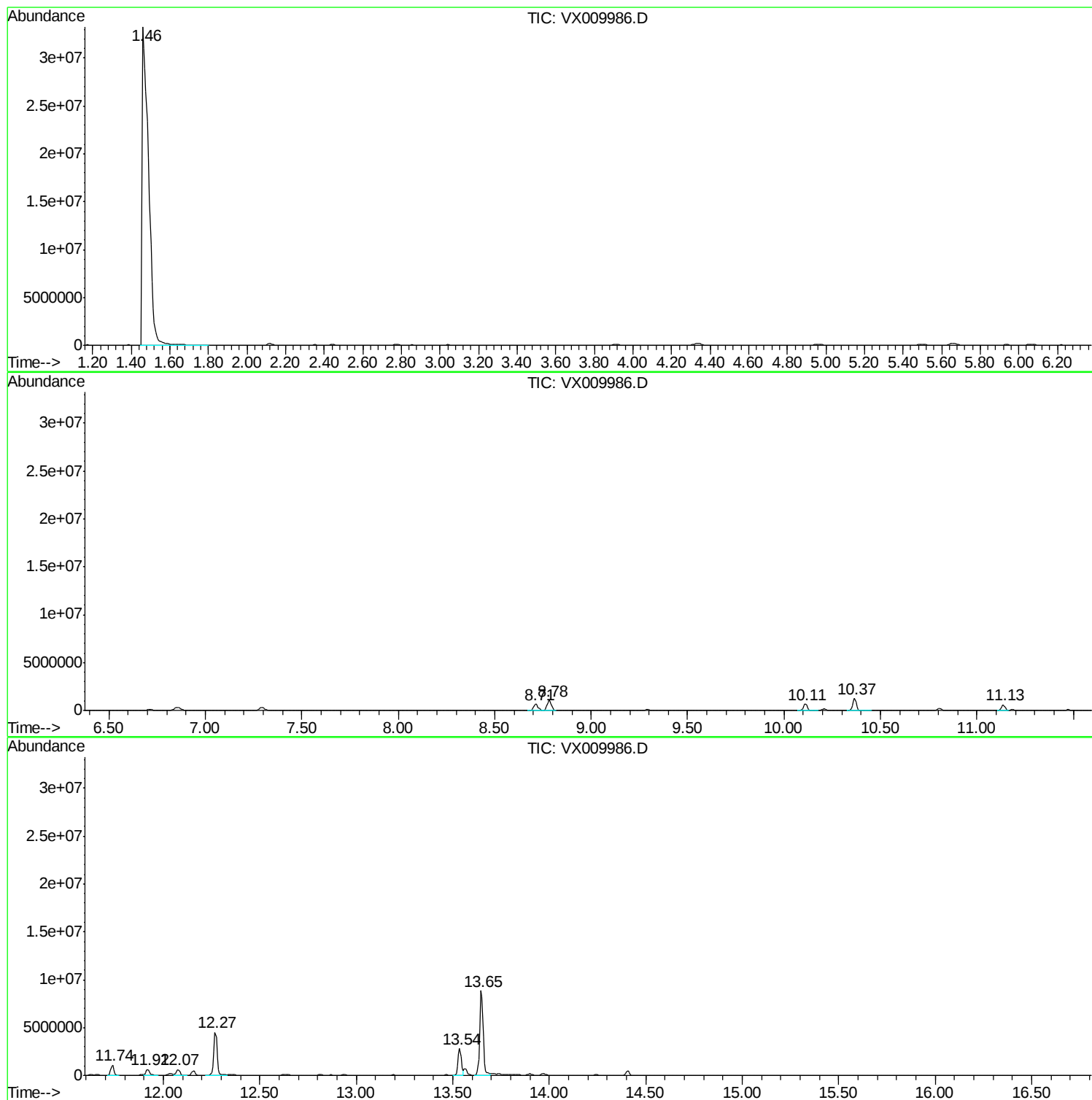
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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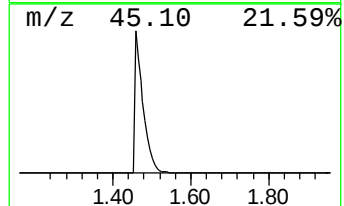
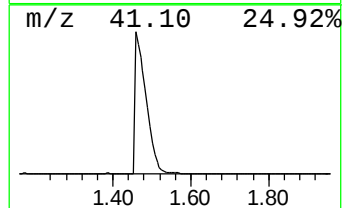
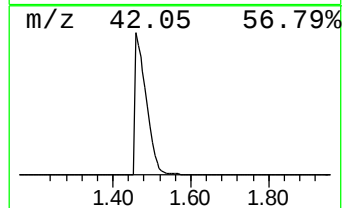
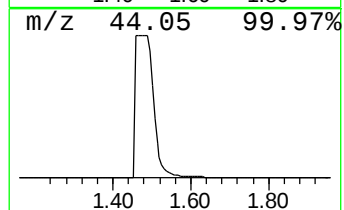
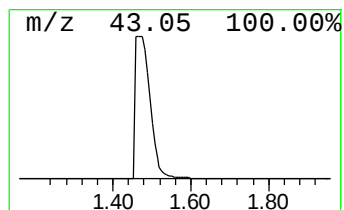
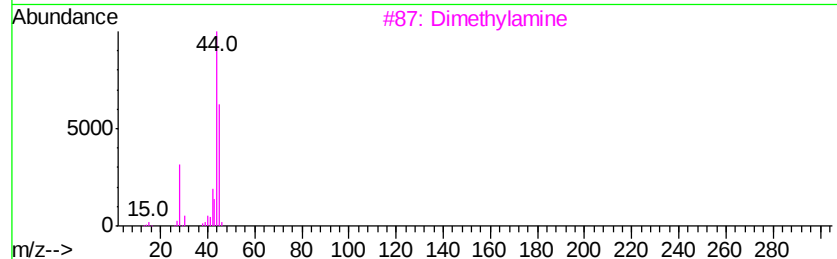
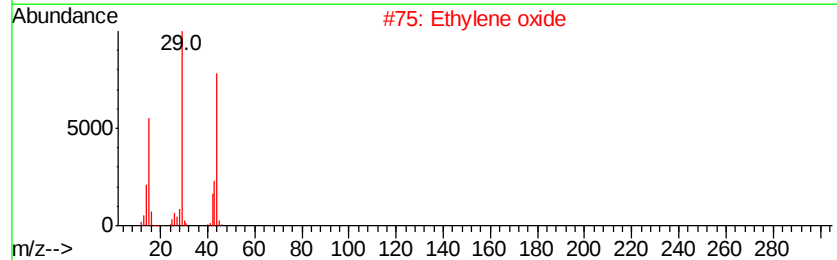
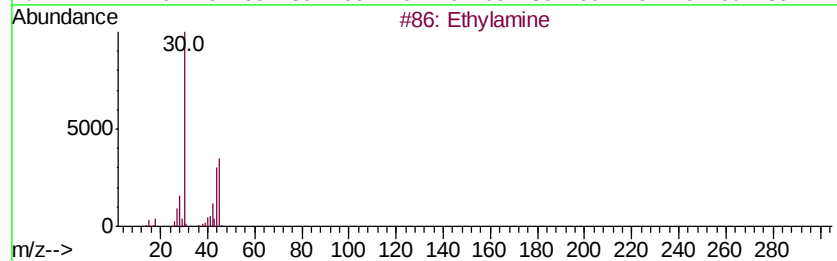
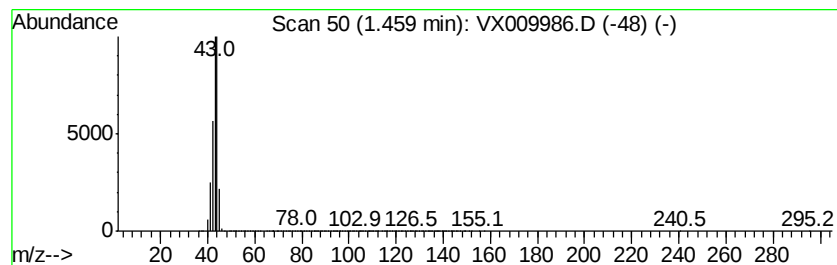
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052819W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethylamine Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.46	3632.18 ug/l	76009900	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylamine		45	C2H7N	000075-04-7	4
2	Ethylene oxide		44	C2H4O	000075-21-8	3
3	Dimethylamine		45	C2H7N	000124-40-3	3
4	Propane		44	C3H8	000074-98-6	3
5	Ketene		42	C2H2O	000463-51-4	3



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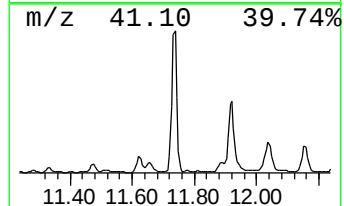
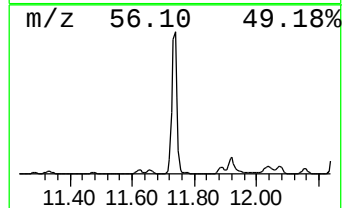
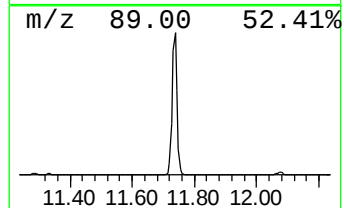
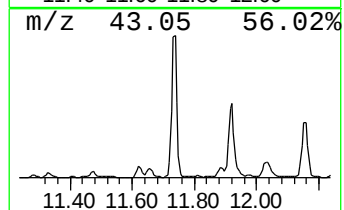
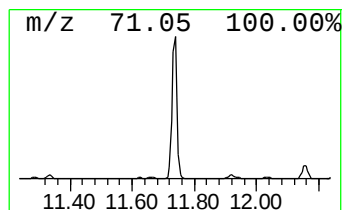
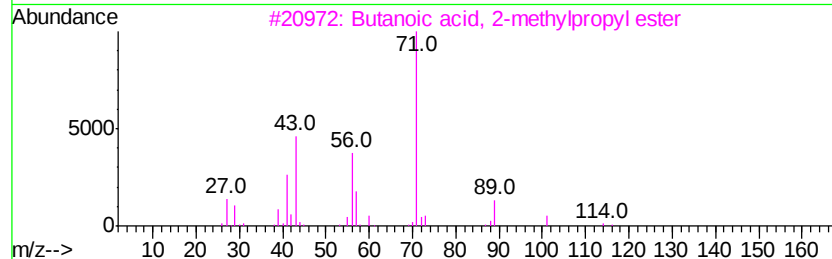
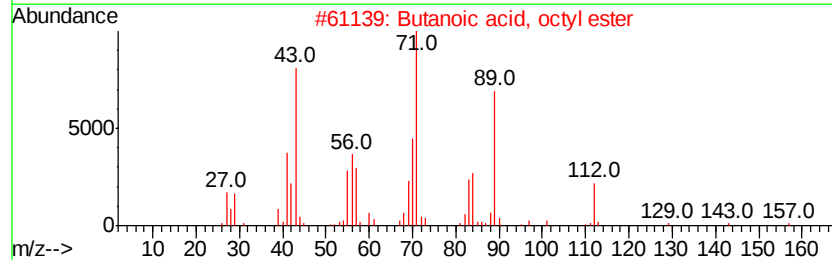
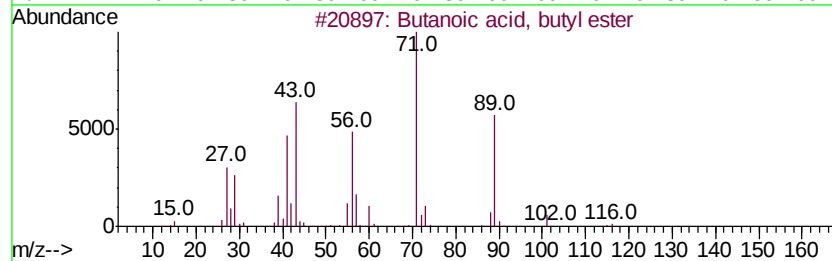
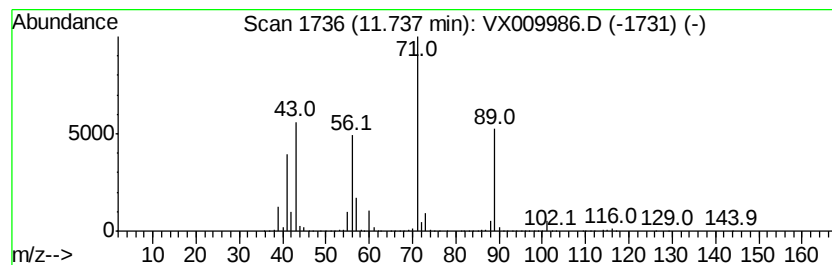
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Butanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.74	77.38 ug/l	1255310	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	90	
2	Butanoic acid, octyl ester	200	C12H24O2	000110-39-4	72	
3	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72	
4	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	72	
5	Propanoic acid, 2-methyl-, butyl...	144	C8H16O2	000097-87-0	56	



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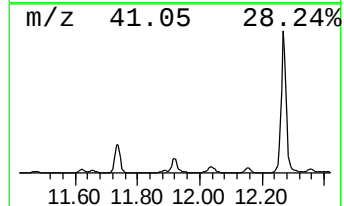
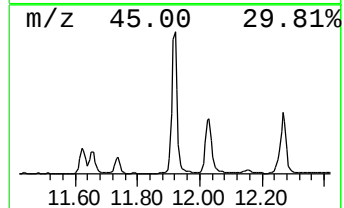
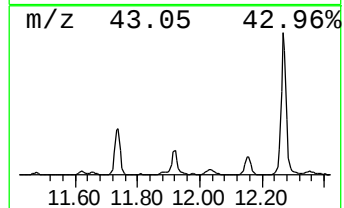
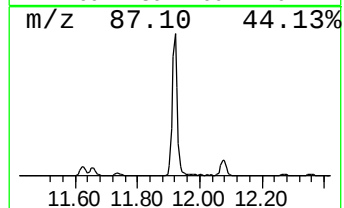
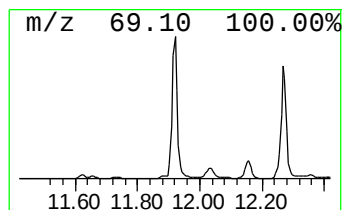
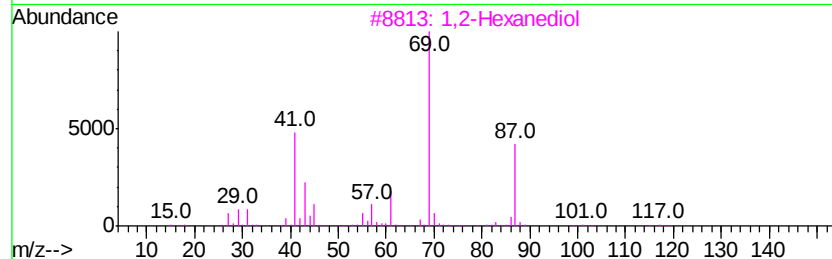
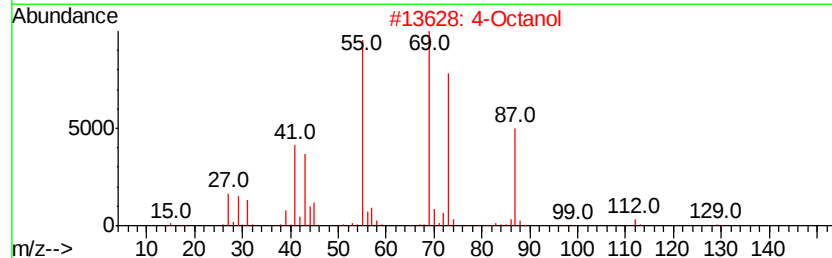
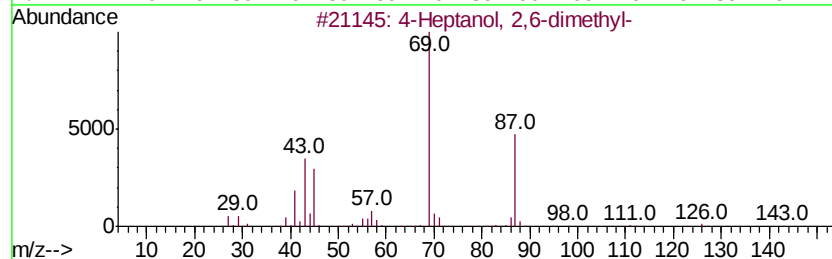
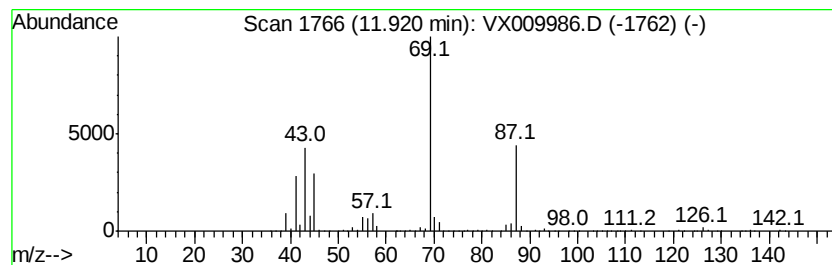
Instrument :
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Peak Number 3 4-Heptanol, 2,6-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.92	49.30 ug/l	799841	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	90
2	4-Octanol	130	C8H18O	000589-62-8	72
3	1,2-Hexanediol	118	C6H14O2	006920-22-5	72
4	5-Nonanol	144	C9H20O	000623-93-8	72
5	3-Hexanol, 2,5-dimethyl-	130	C8H18O	019550-07-3	72



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Instrument :
MSVOA_X
ClientSampled :
COMP-3

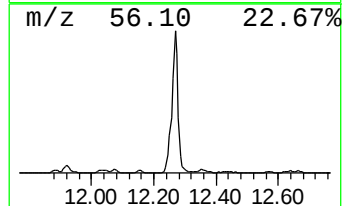
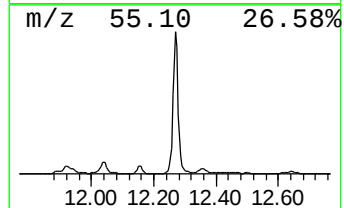
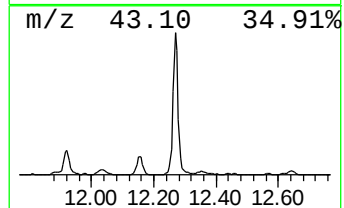
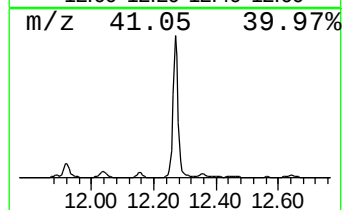
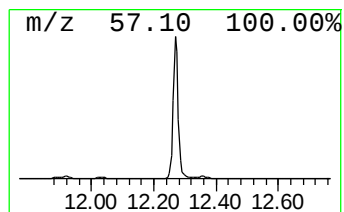
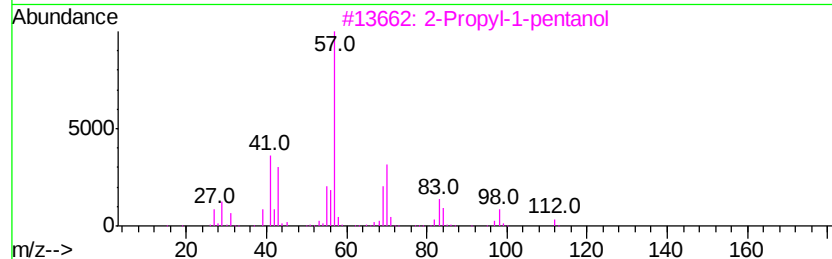
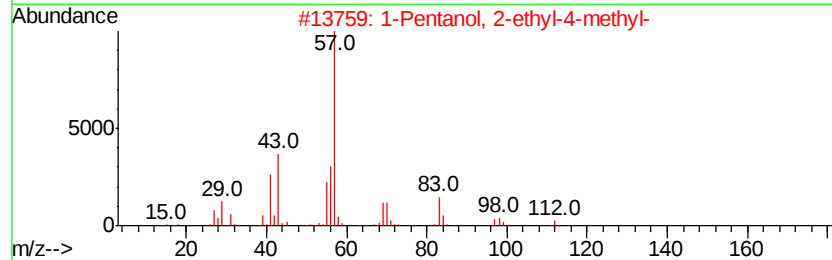
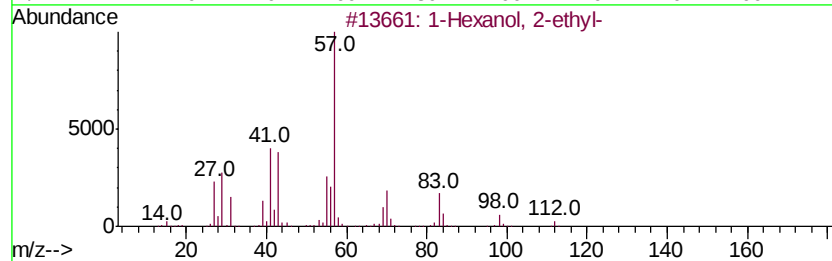
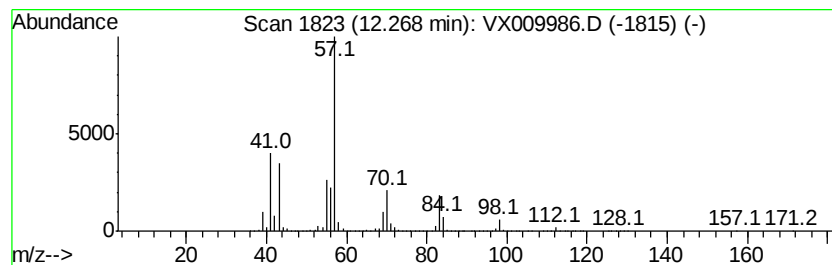
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	351.18 ug/l	5697200	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	78
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
3		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	42
5		2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	42



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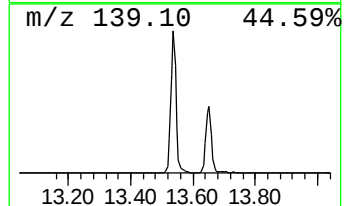
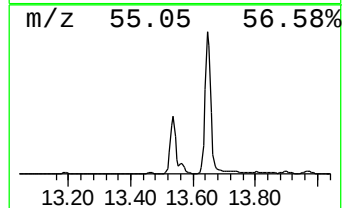
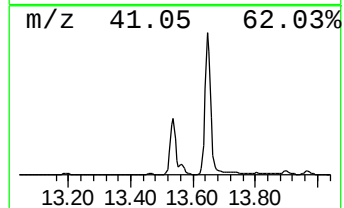
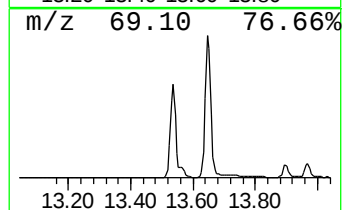
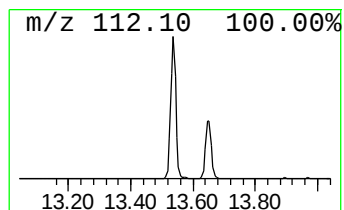
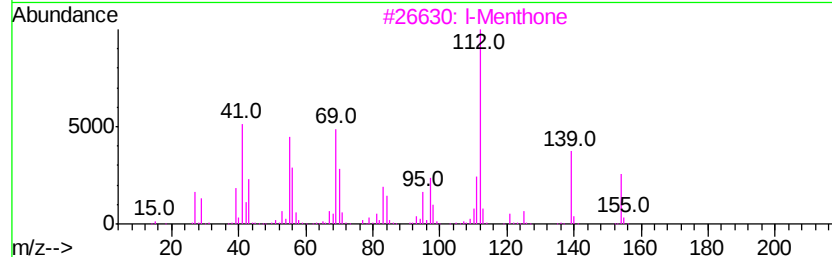
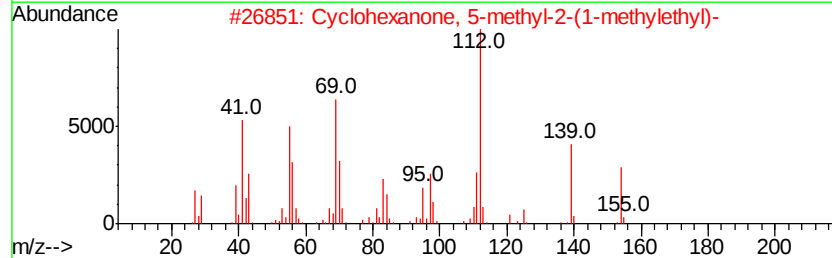
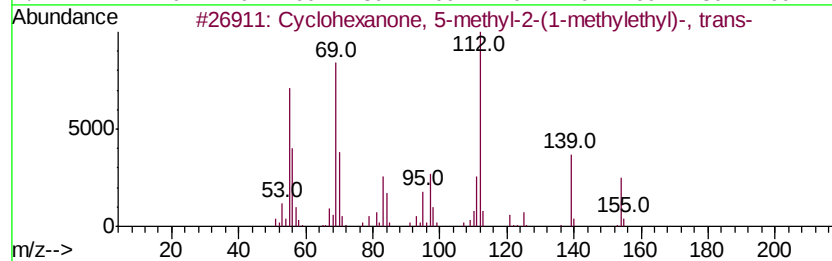
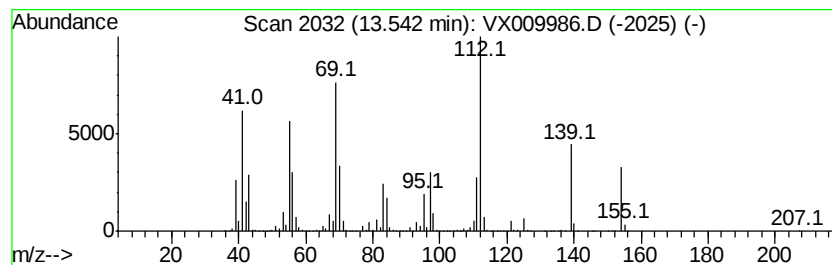
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclohexanone, 5-methyl-2-(... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.54	210.94 ug/l	3422020	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000089-80-5	98
2		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	010458-14-7	98
3		l-Menthone	154	C10H18O	014073-97-3	98
4		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	001196-31-2	98
5		Cyclohexanone, 5-methyl-2-(1-met...	154	C10H18O	000491-07-6	98



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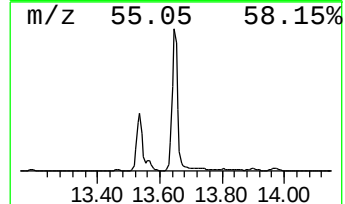
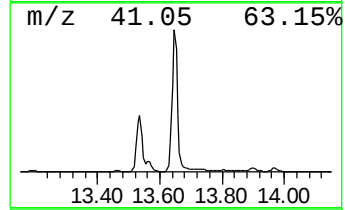
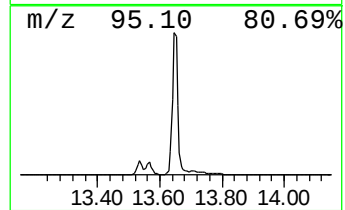
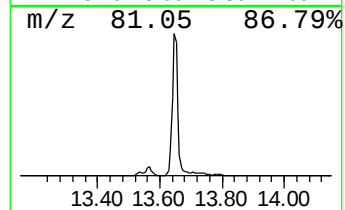
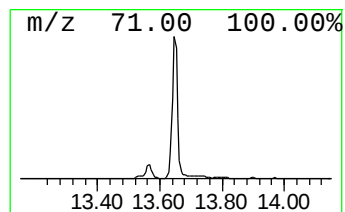
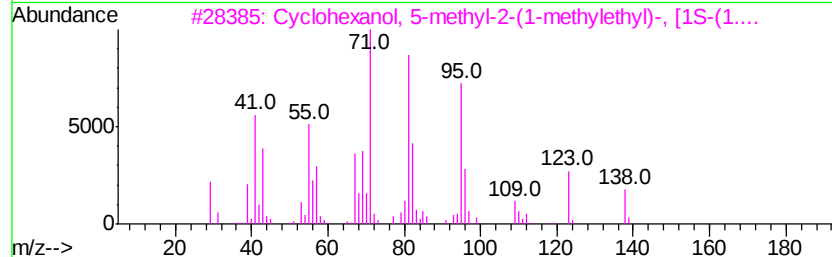
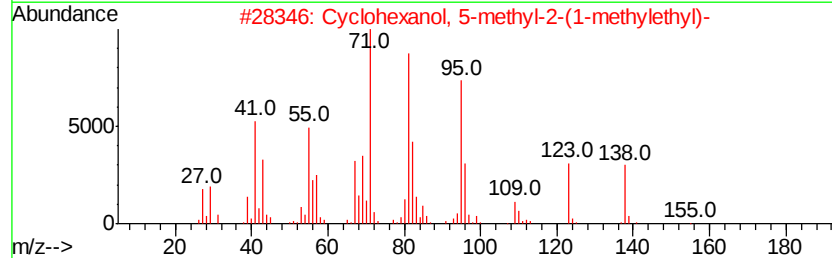
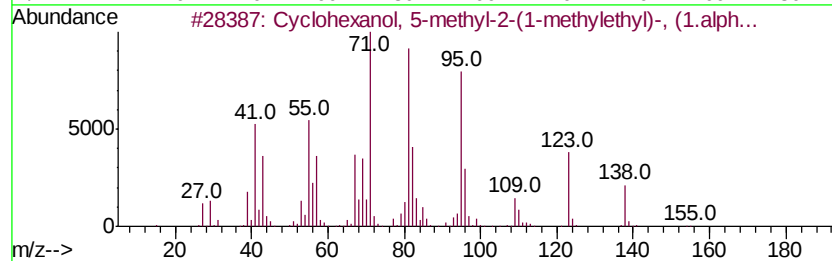
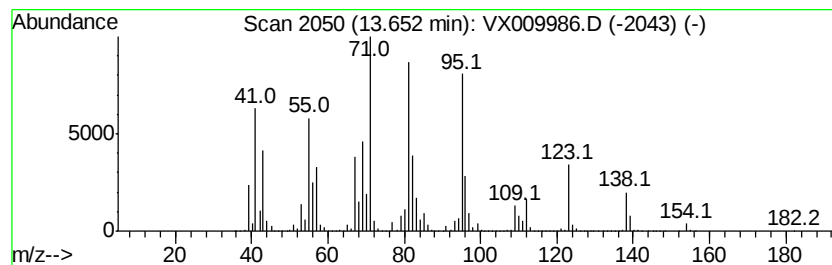
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Cyclohexanol, 5-methyl-2-(1... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.65	689.89 ug/l	11192000	1,4-Dichlorobenzene-d4	12.08

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	015356-70-4	91
2		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	001490-04-6	91
3		Cyclohexanol, 5-methyl-2-(1-meth...	156	C10H20O	002216-52-6	91
4		Levomenthol	156	C10H20O	002216-51-5	91
5		dl-Menthol	156	C10H20O	000089-78-1	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX053119\
Data File : VX009986.D
Acq On : 31 May 2019 15:37
Operator : JC/SP
Sample : K2964-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
COMP-3

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethylamine	1.46	3632.2	ug/l	76009900	1	5.66	1046340	50.0
Butanoic acid, bu...	11.74	77.4	ug/l	1255310	4	12.08	811150	50.0
4-Heptanol, 2,6-d...	11.92	49.3	ug/l	799841	4	12.08	811150	50.0
1-Hexanol, 2-ethyl-	12.27	351.2	ug/l	5697200	4	12.08	811150	50.0
Cyclohexanone, 5-...	13.54	210.9	ug/l	3422020	4	12.08	811150	50.0
Cyclohexanol, 5-m...	13.65	689.9	ug/l	11192000	4	12.08	811150	50.0