

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX021519\
 Data File : VX007542.D
 Acq On : 14 Feb 2019 13:42
 Operator : JC/SP
 Sample : K1458-10
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 WC-6

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\82X020119W.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	1.605	67	74	79	rVB2	21204	38775	1.27%	0.168%
2	2.446	206	212	218	rBV	29633	50417	1.65%	0.218%
3	2.861	273	280	289	rBV	177307	328268	10.76%	1.419%
4	5.500	703	713	727	rBV	291039	825072	27.05%	3.567%
5	5.665	727	740	758	rVB2	459480	1304770	42.77%	5.640%
6	6.067	796	806	818	rBV	290016	749816	24.58%	3.241%
7	6.464	863	871	882	rVB3	21713	54506	1.79%	0.236%
8	6.860	926	936	946	rBV	710476	1684507	55.22%	7.282%
9	7.549	1044	1049	1054	rBV	21372	38534	1.26%	0.167%
10	7.726	1075	1078	1083	rVV2	24044	39930	1.31%	0.173%
11	7.878	1095	1103	1116	rBV	1802084	3050719	100.00%	13.188%
12	8.616	1218	1224	1233	rBV	440510	670038	21.96%	2.897%
13	8.713	1233	1240	1249	rBV	1556021	2392940	78.44%	10.345%
14	9.018	1285	1290	1297	rVB	34201	55949	1.83%	0.242%
15	9.305	1331	1337	1344	rBV	286600	408799	13.40%	1.767%
16	9.372	1344	1348	1350	rVV	39075	51747	1.70%	0.224%
17	9.402	1350	1353	1357	rVV	100405	143053	4.69%	0.618%
18	9.439	1357	1359	1363	rVB	36941	45708	1.50%	0.198%
19	9.542	1370	1376	1383	rBV	1780138	2189193	71.76%	9.464%
20	9.640	1387	1392	1401	rVB	91824	119349	3.91%	0.516%
21	9.969	1441	1446	1456	rBV	1566062	1912378	62.69%	8.267%
22	10.109	1462	1469	1476	rBV	1536165	2130666	69.84%	9.211%
23	10.561	1539	1543	1547	rBV	24554	30749	1.01%	0.133%
24	10.695	1560	1565	1571	rBV	78644	97963	3.21%	0.423%
25	11.134	1631	1637	1645	rBV	1301323	1658287	54.36%	7.169%
26	11.804	1743	1747	1751	rBV	28938	37410	1.23%	0.162%
27	12.079	1786	1792	1798	rBV	1656827	2036383	66.75%	8.803%
28	12.298	1821	1828	1835	rVB2	32885	57166	1.87%	0.247%
29	13.347	1991	2000	2005	rBV2	57159	84217	2.76%	0.364%
30	13.481	2017	2022	2028	rVB2	35301	44643	1.46%	0.193%
31	13.834	2070	2080	2087	rBV	392583	489351	16.04%	2.115%
32	14.286	2148	2154	2158	rBV3	25521	46995	1.54%	0.203%
33	14.694	2214	2221	2226	rBV	96887	125899	4.13%	0.544%
34	14.840	2240	2245	2250	rBV	106004	138184	4.53%	0.597%

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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

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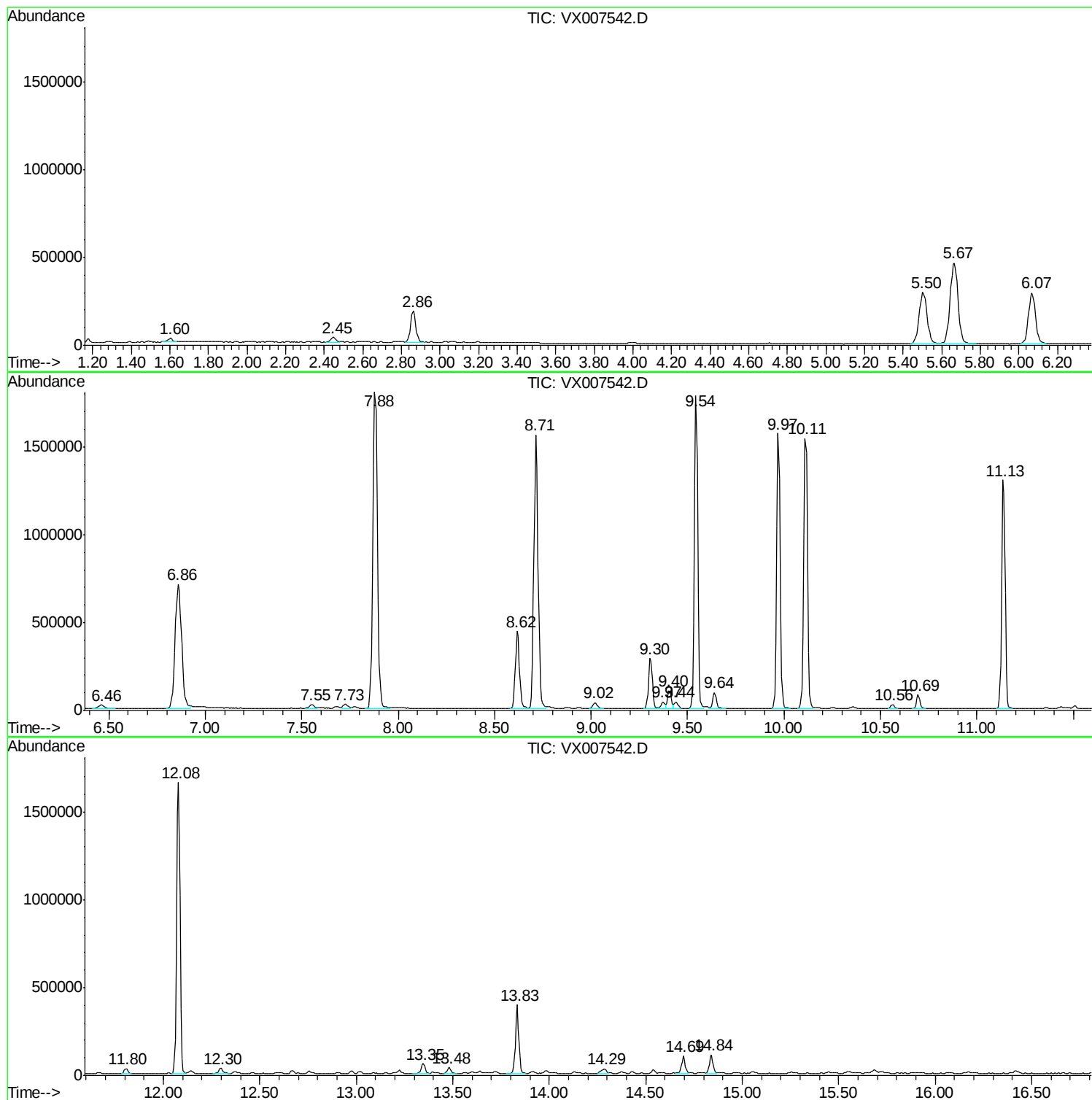
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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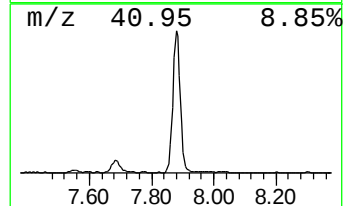
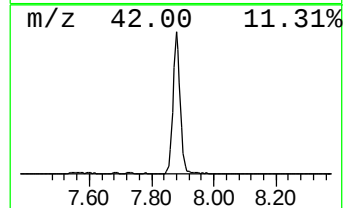
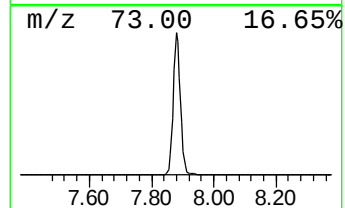
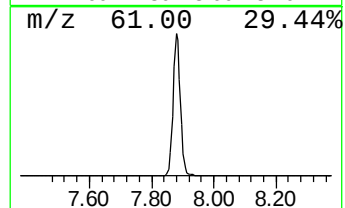
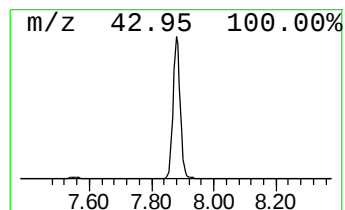
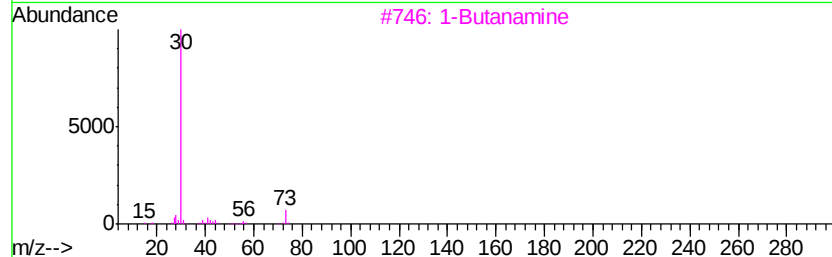
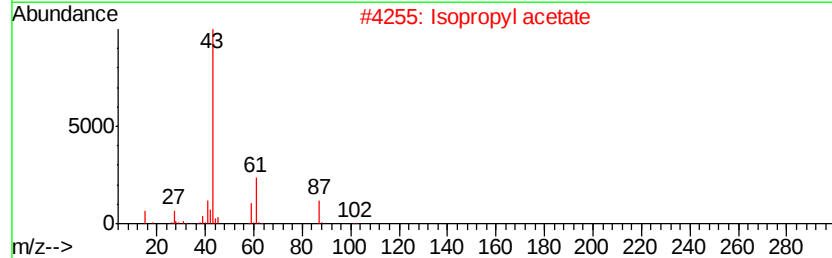
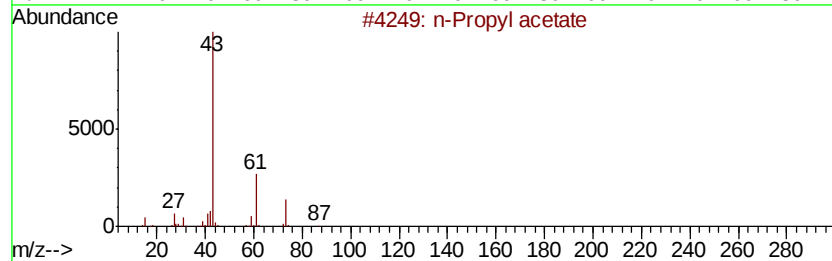
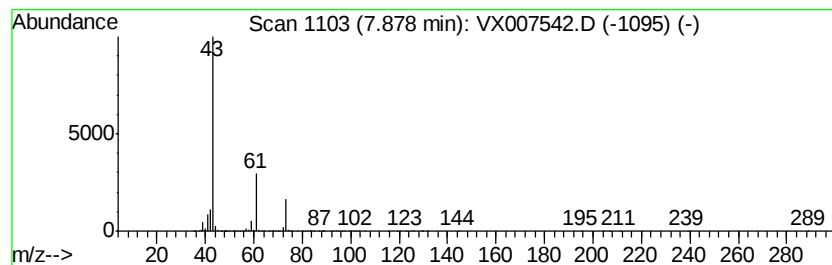
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	90.55 ug/l	3050720	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	83
2		Isopropyl acetate	102	C5H10O2	000108-21-4	36
3		1-Butanamine	73	C4H11N	000109-73-9	7
4		Isobutylamine	73	C4H11N	000078-81-9	4
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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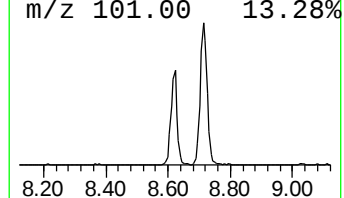
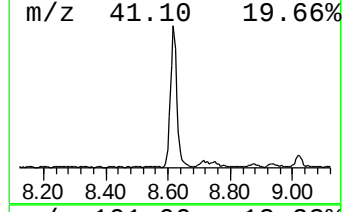
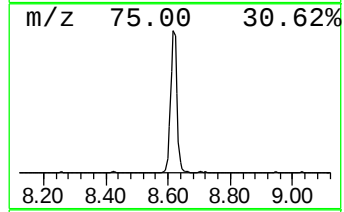
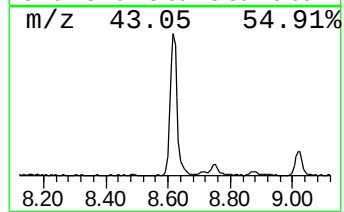
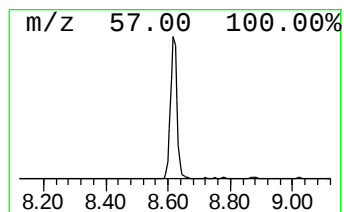
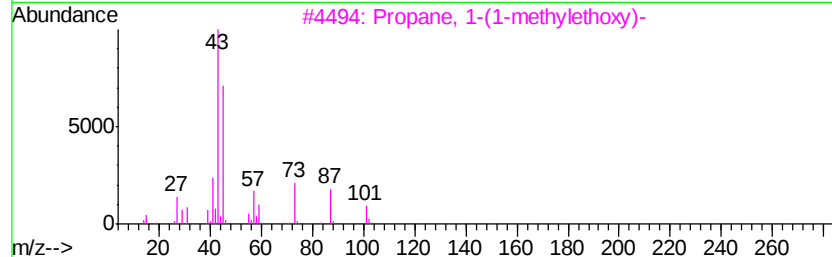
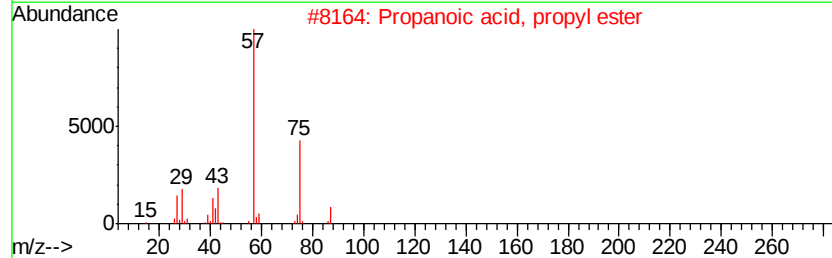
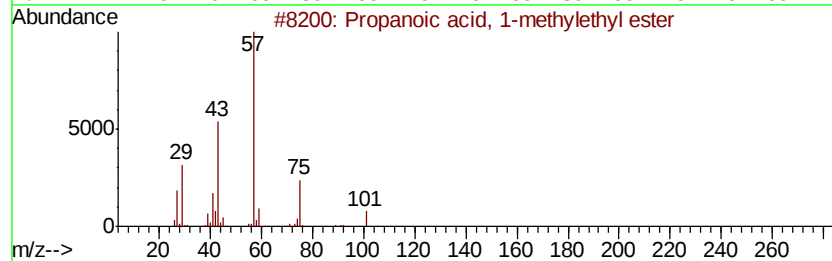
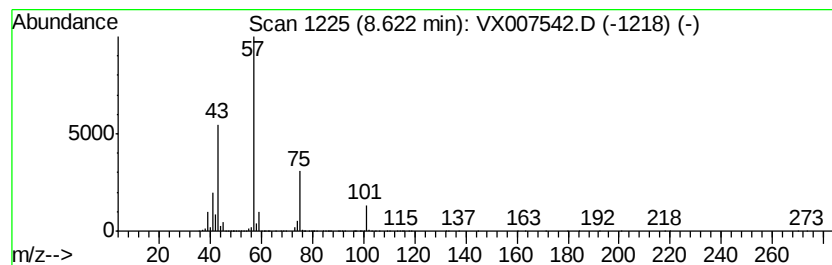
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	15.72 ug/l	670038	Chlorobenzene-d5	10.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83	
2	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	59	
3	Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	23	
4	Azetidine	57	C3H7N	000503-29-7	12	
5	(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9	



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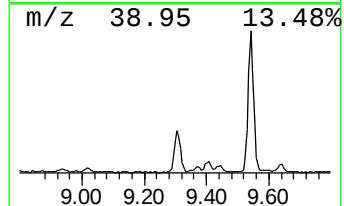
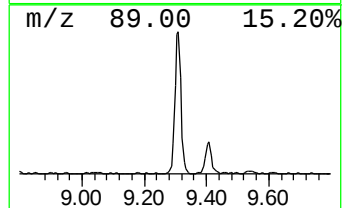
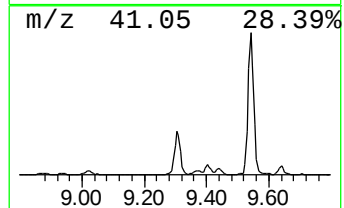
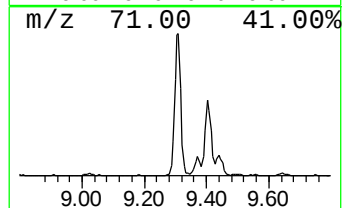
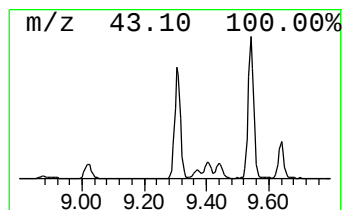
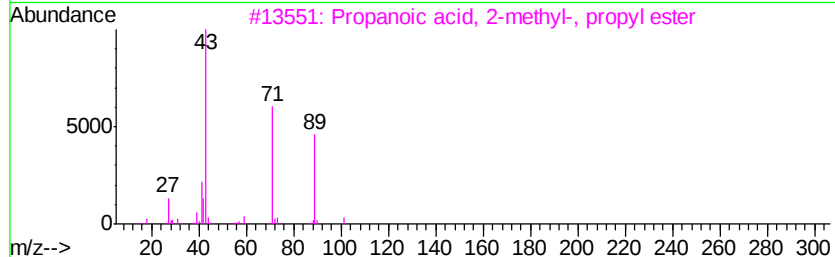
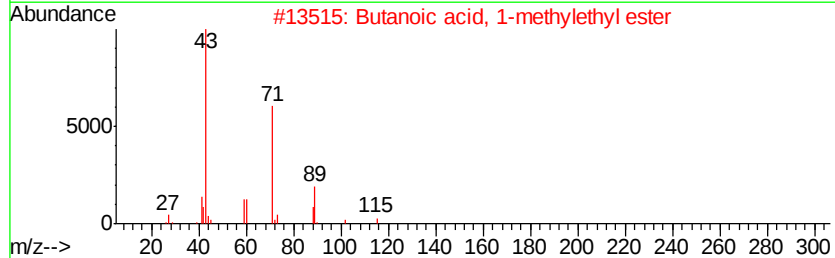
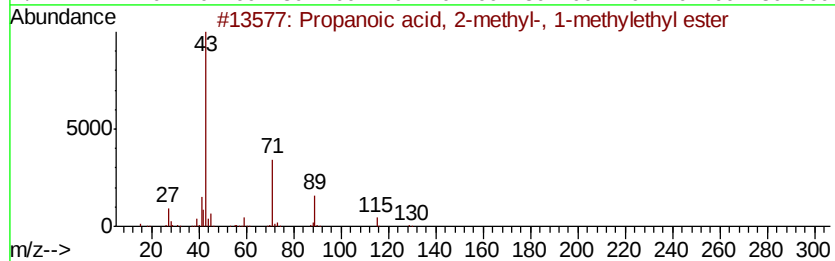
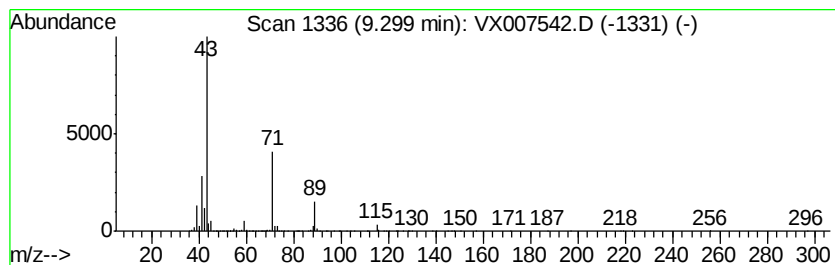
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	9.59 ug/l	408799	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	72
3		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	64
4		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	42
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	38



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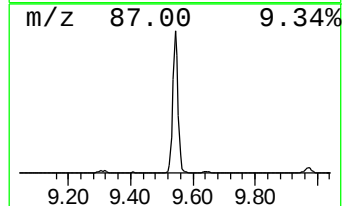
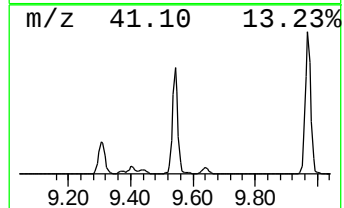
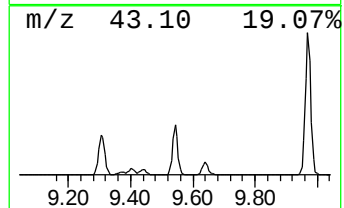
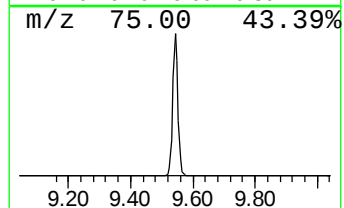
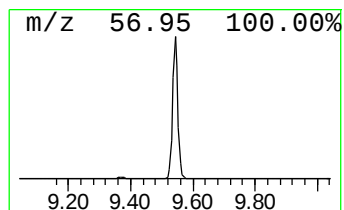
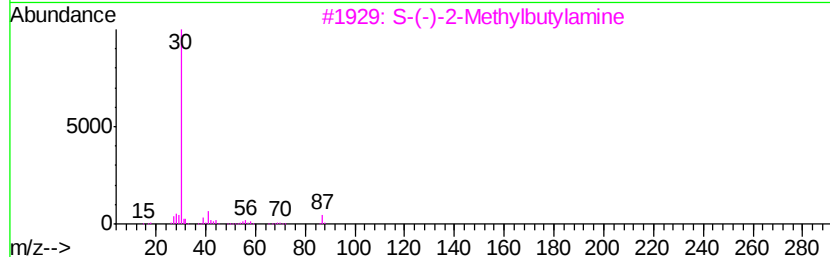
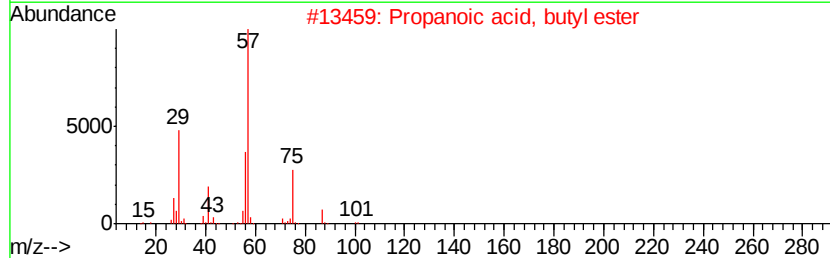
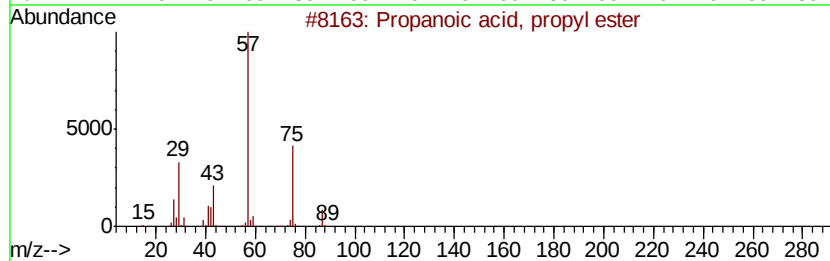
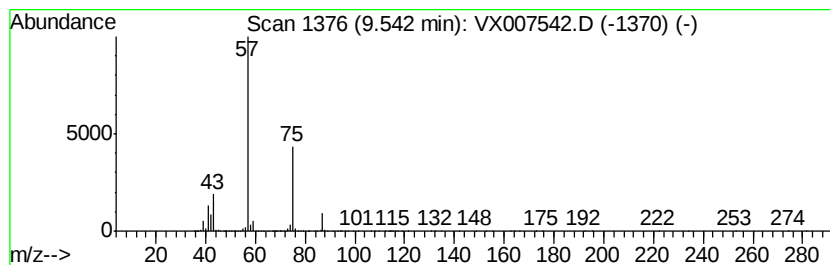
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	51.37 ug/l	2189190	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2		Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	28
3		S-(-)-2-Methylbutylamine	87	C5H13N	020626-52-2	9
4		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
5		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7



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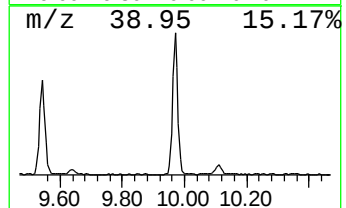
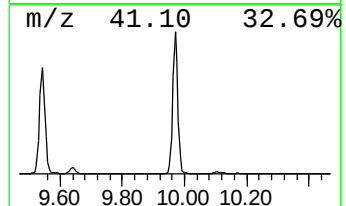
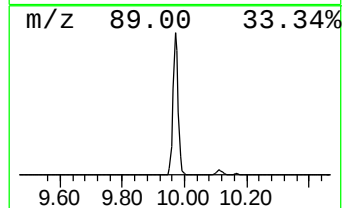
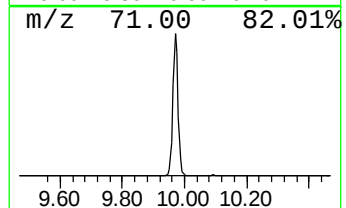
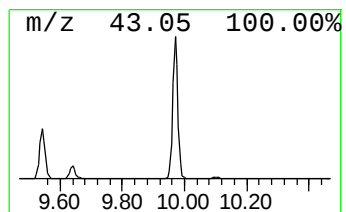
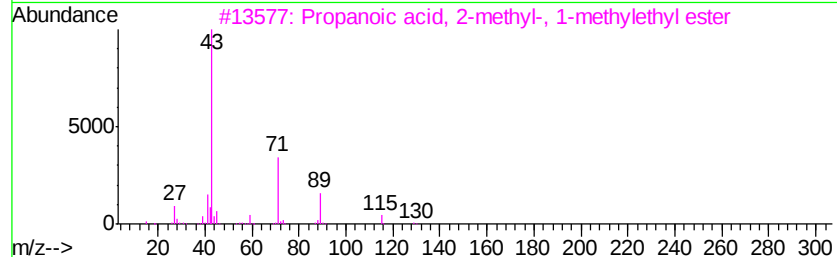
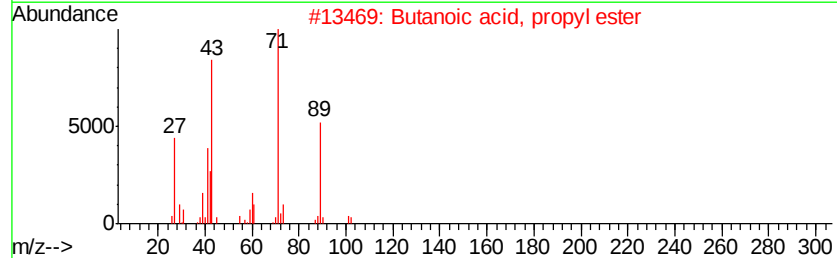
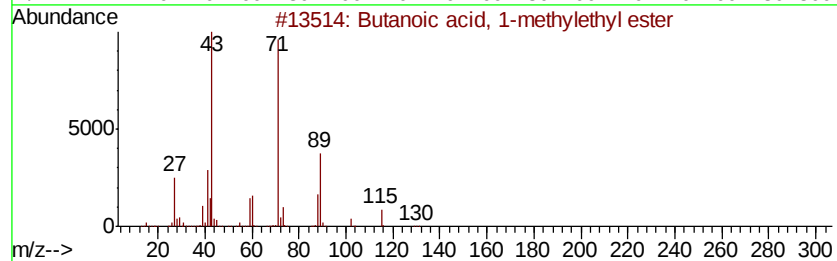
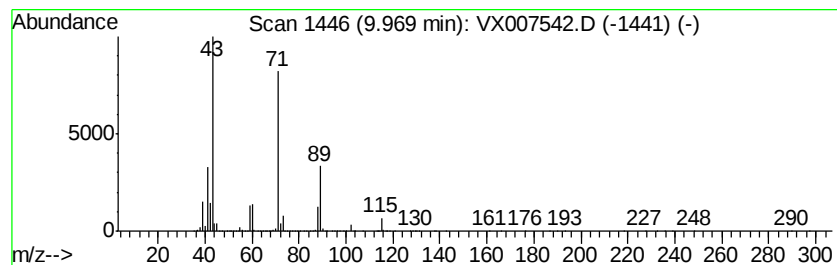
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Peak Number 5 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	44.88 ug/l	1912380	Chlorobenzene-d5	10.11

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
3		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
4		Ethane-1,1-diol dibutanoate	202	C10H18O4	025572-25-2	50
5		Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX021519\
Data File : VX007542.D
Acq On : 14 Feb 2019 13:42
Operator : JC/SP
Sample : K1458-10
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
WC-6

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X020119W.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
n-Propyl acetate	7.88	90.5	ug/l	3050720	2	6.86	1684510	50.0
Propanoic acid, 1...	8.62	15.7	ug/l	670038	3	10.11	2130670	50.0
Propanoic acid, 2...	9.30	9.6	ug/l	408799	3	10.11	2130670	50.0
Propanoic acid, p...	9.54	51.4	ug/l	2189190	3	10.11	2130670	50.0
Butanoic acid, 1...	9.97	44.9	ug/l	1912380	3	10.11	2130670	50.0