

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121118\
 Data File : VX006432.D
 Acq On : 11 Dec 2018 20:24
 Operator : JC/MD
 Sample : J6331-42
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 TP-7

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\82X112918W.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	1.617	66	76	84	rBV6	42411	102114	2.32%	0.286%
2	2.861	273	280	295	rBV	1341009	2516401	57.07%	7.041%
3	5.507	701	714	728	rBV	426870	1216875	27.60%	3.405%
4	5.665	729	740	755	rVB	743134	2076836	47.10%	5.811%
5	6.068	793	806	816	rBV	417314	1072093	24.31%	3.000%
6	6.458	864	870	880	rVB2	34279	88049	2.00%	0.246%
7	6.860	924	936	947	rBV	1085207	2558325	58.02%	7.158%
8	7.549	1044	1049	1054	rBV	23688	46172	1.05%	0.129%
9	7.634	1054	1063	1069	rBV2	37522	99853	2.26%	0.279%
10	7.726	1074	1078	1083	rVV	34139	64715	1.47%	0.181%
11	7.884	1096	1104	1117	rBV	2535085	4409604	100.00%	12.338%
12	8.616	1218	1224	1234	rBV	503684	783917	17.78%	2.193%
13	8.713	1234	1240	1250	rBV	2239205	3478544	78.89%	9.733%
14	9.018	1284	1290	1297	rVB	59704	90037	2.04%	0.252%
15	9.311	1331	1338	1344	rBV	299674	440857	10.00%	1.233%
16	9.372	1344	1348	1350	rVV	44961	61798	1.40%	0.173%
17	9.408	1350	1354	1357	rVV	134661	192300	4.36%	0.538%
18	9.439	1357	1359	1365	rVB	39886	49614	1.13%	0.139%
19	9.543	1371	1376	1387	rVV	2252045	2907756	65.94%	8.136%
20	9.640	1387	1392	1400	rVB	180035	229111	5.20%	0.641%
21	9.969	1441	1446	1457	rBV	1716556	2175813	49.34%	6.088%
22	10.116	1459	1470	1477	rBV	2169446	3045399	69.06%	8.521%
23	10.360	1504	1510	1515	rBV	44313	66879	1.52%	0.187%
24	10.695	1560	1565	1569	rBV	113993	142149	3.22%	0.398%
25	10.737	1569	1572	1579	rVB	34986	47951	1.09%	0.134%
26	11.140	1632	1638	1644	rBV	1865968	2462171	55.84%	6.889%
27	11.432	1681	1686	1688	rBV	33563	45922	1.04%	0.128%
28	11.804	1743	1747	1753	rBV	105579	139098	3.15%	0.389%
29	12.079	1786	1792	1799	rBV	2495702	3049357	69.15%	8.532%
30	12.140	1799	1802	1807	rVB	33627	44366	1.01%	0.124%
31	12.298	1821	1828	1835	rBV2	60945	98726	2.24%	0.276%
32	12.371	1835	1840	1847	rVB3	33937	51303	1.16%	0.144%
33	12.670	1884	1889	1892	rBV	42715	53059	1.20%	0.148%
34	12.755	1899	1903	1911	rBV2	31577	52722	1.20%	0.148%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-7

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\82X112918W.M
Title : SW846 8260

35	12.975	1934	1939	1943	rBV	34892	44574	1.01%	0.125%
36	13.347	1996	2000	2006	rVB2	92328	133299	3.02%	0.373%
37	13.481	2017	2022	2029	rVB	45187	63175	1.43%	0.177%
38	13.834	2073	2080	2087	rVB	638558	812975	18.44%	2.275%
39	14.286	2147	2154	2161	rVB3	53792	92364	2.09%	0.258%
40	14.542	2190	2196	2201	rBV2	38385	54012	1.22%	0.151%
41	14.694	2211	2221	2226	rBV	142552	206008	4.67%	0.576%
42	14.840	2240	2245	2249	rBV	115960	150029	3.40%	0.420%
43	15.548	2354	2361	2367	rBV2	30684	57790	1.31%	0.162%
44	15.688	2378	2384	2387	rBV	44589	69490	1.58%	0.194%
45	15.724	2387	2390	2397	rVB2	27923	46008	1.04%	0.129%
46	16.419	2496	2504	2512	rBV3	22619	51465	1.17%	0.144%

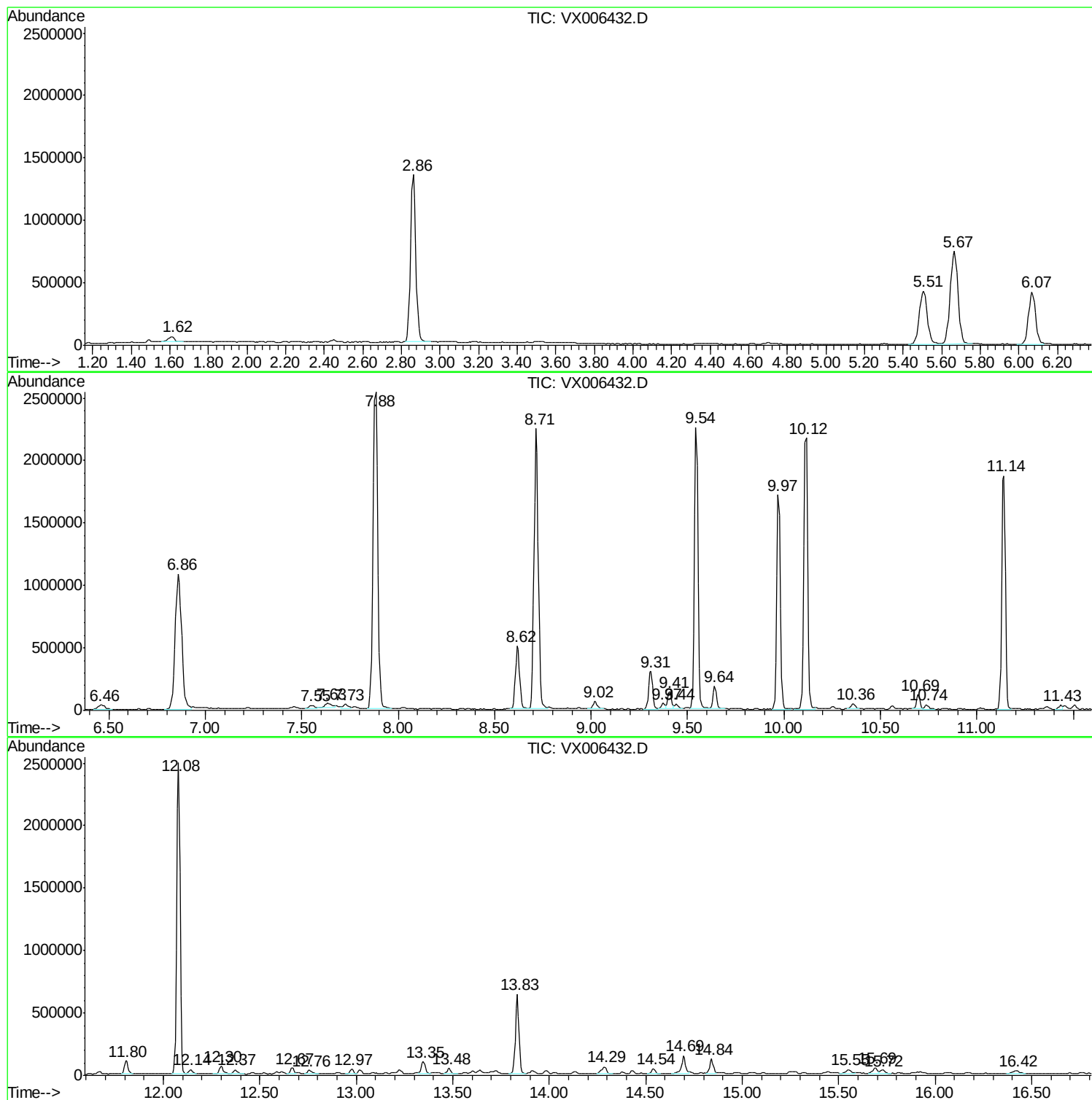
Sum of corrected areas: 35741075

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-7

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
 Data File : VX006432.D
 Acq On : 11 Dec 2018 20:24
 Operator : JC/MD
 Sample : J6331-42
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

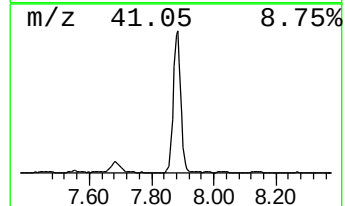
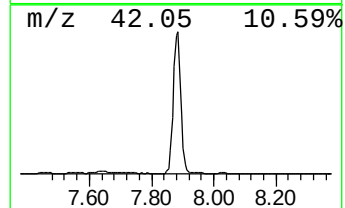
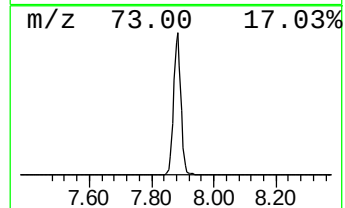
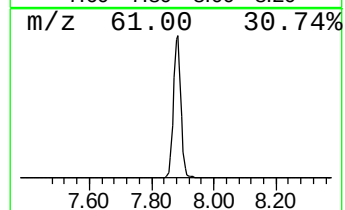
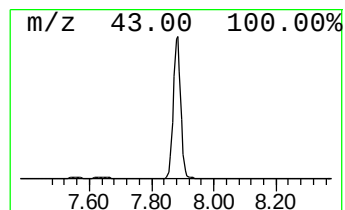
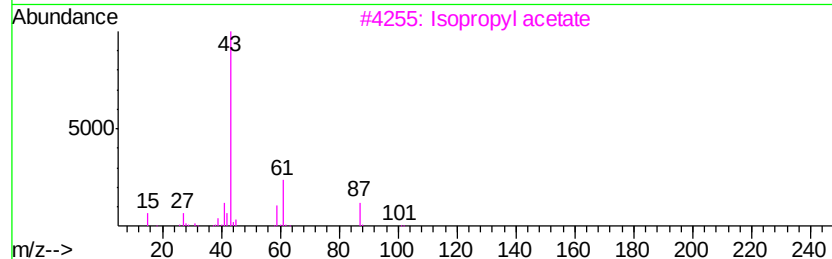
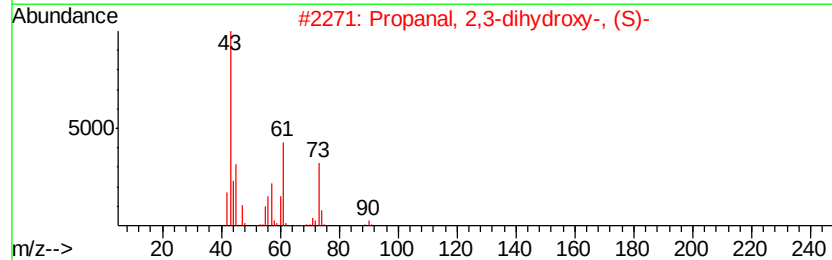
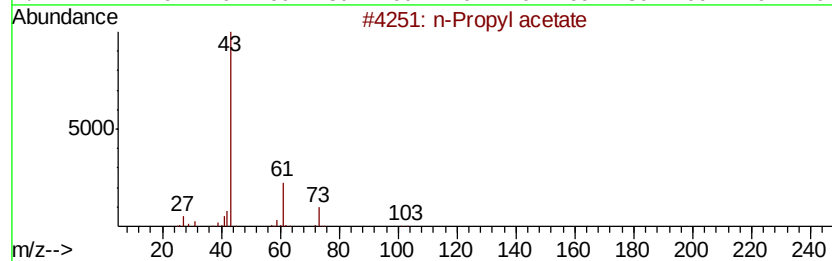
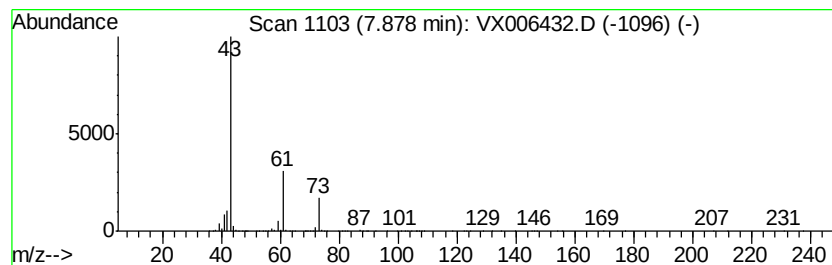
Instrument :
 MSVOA_X
 ClientSampleId :
 TP-7

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
 Quant Title : SW846 8260

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	86.18 ug/l	4409600	1,4-Difluorobenzene	6.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	n-Propyl acetate	102 C5H10O2	000109-60-4	83
2	Propanal, 2,3-dihydroxy-, (S)-	90 C3H6O3	000497-09-6	36
3	Isopropyl acetate	102 C5H10O2	000108-21-4	36
4	1-Butanamine	73 C4H11N	000109-73-9	7
5	Isobutylamine	73 C4H11N	000078-81-9	5



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
TP-7

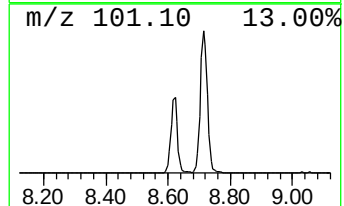
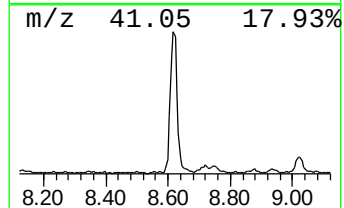
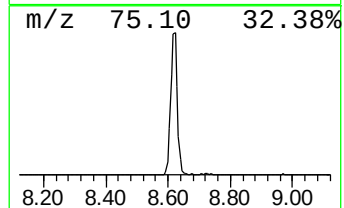
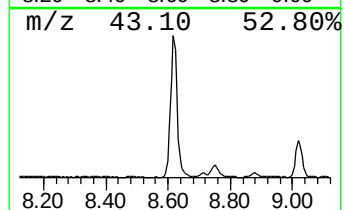
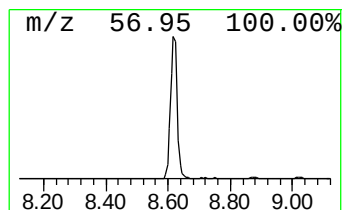
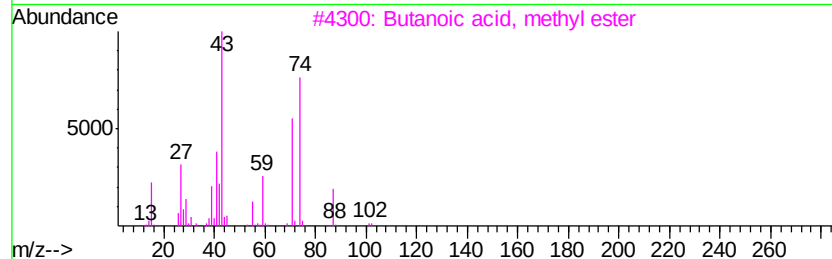
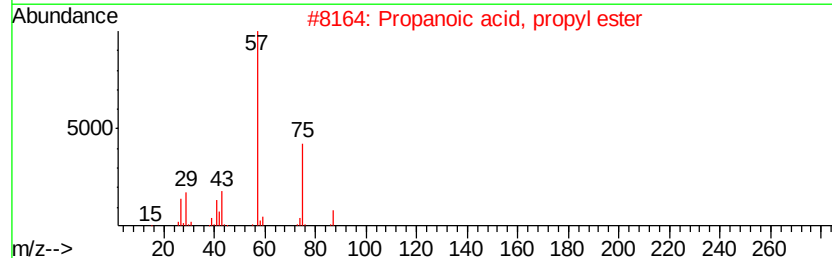
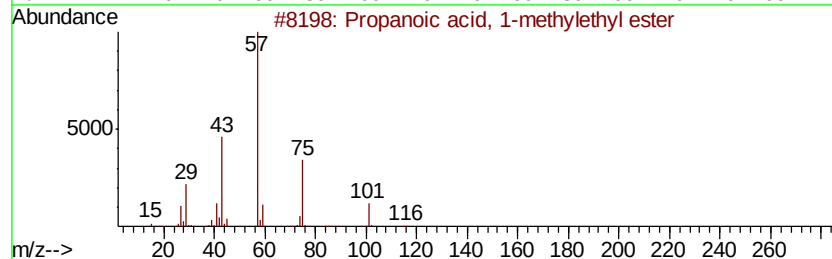
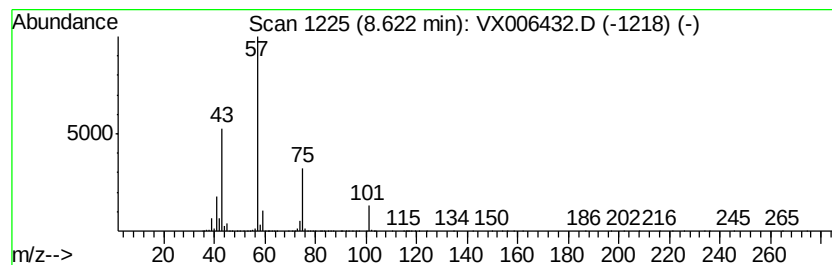
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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	12.87 ug/l	783917	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propanoic acid, 1-methylethyl ester	116	C6H12O2	000637-78-5	83
2		Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	50
3		Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	9
4		o-Isopropylhydroxylamine	75	C3H9NO	1000322-42-6	9
5		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-7

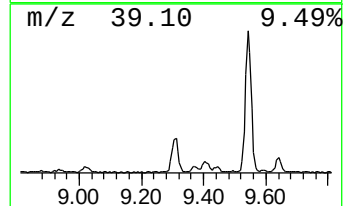
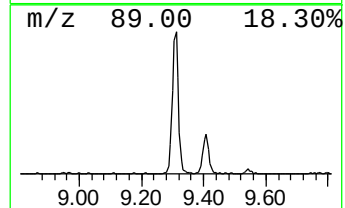
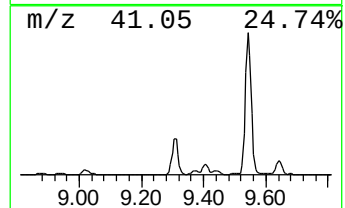
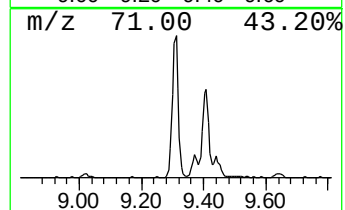
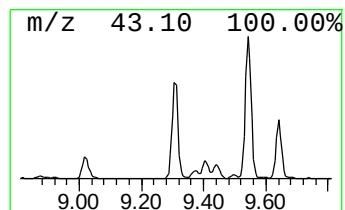
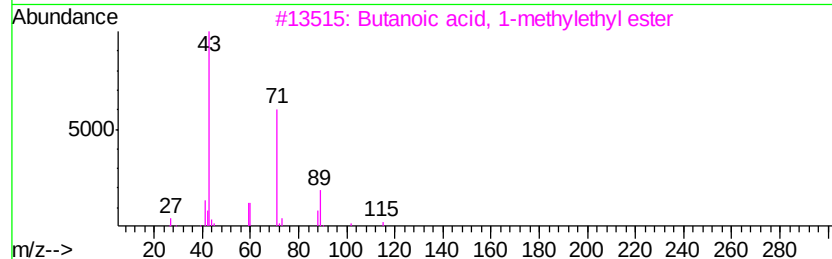
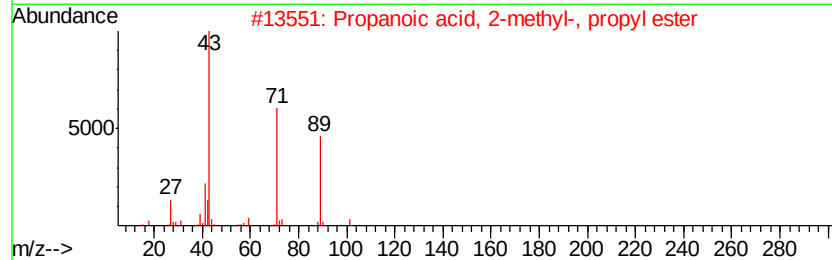
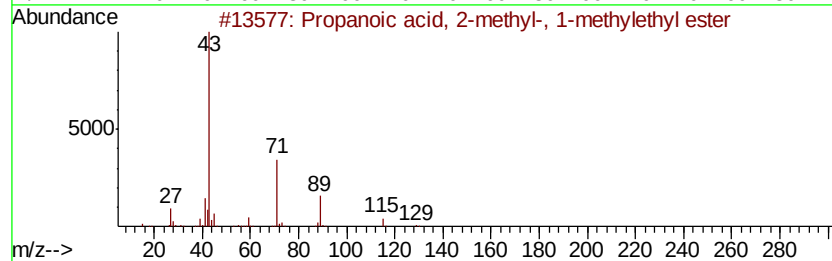
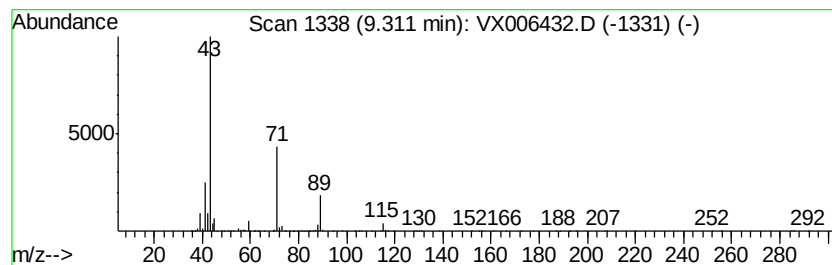
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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.
9.31	7.24 ug/l	440857	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	83
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	64
3		Butanoic acid, 1-methyl-ethyl ester	130	C7H14O2	000638-11-9	50
4		2,3-Hexanedione	114	C6H10O2	003848-24-6	42
5		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-7

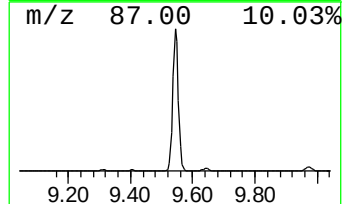
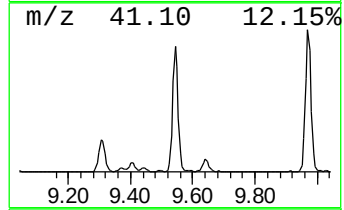
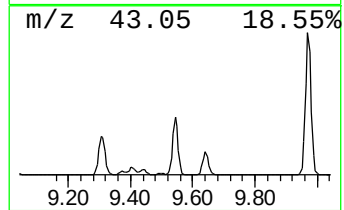
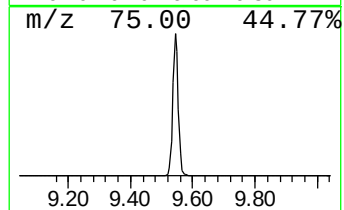
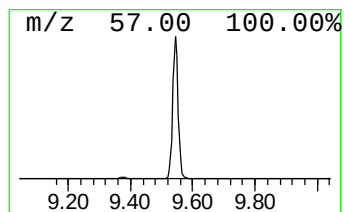
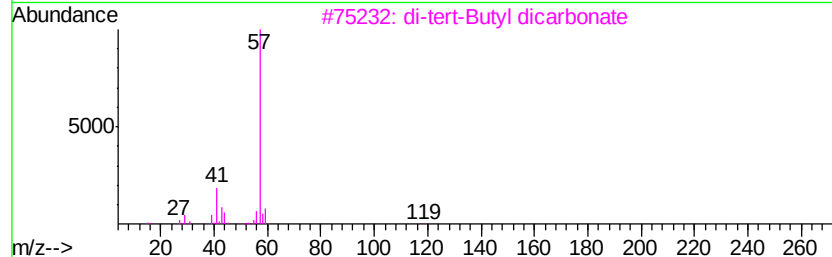
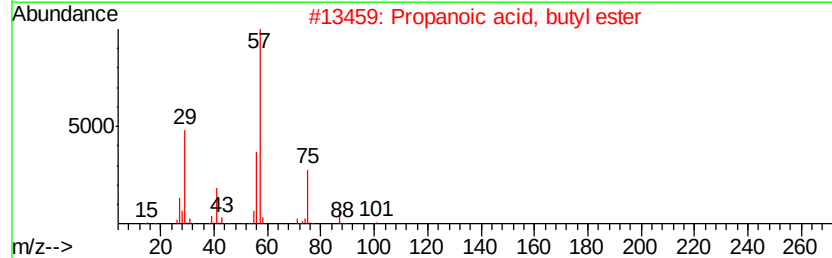
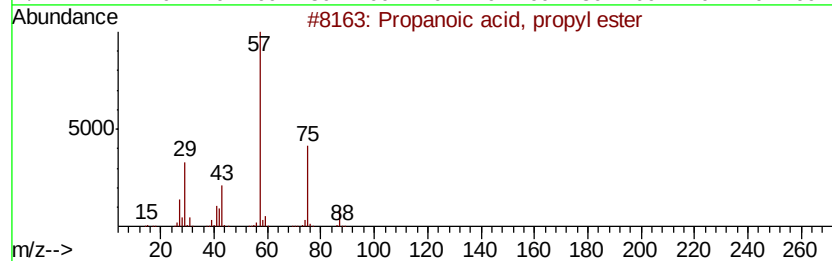
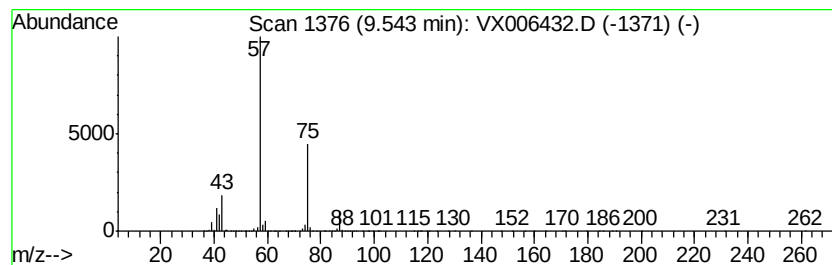
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
Quant Title : SW846 8260

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	47.74 ug/l	2907760	Chlorobenzene-d5	10.12

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		di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4		1-Penten-3-ol	86	C5H10O	000616-25-1	7
5		1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX121118\
 Data File : VX006432.D
 Acq On : 11 Dec 2018 20:24
 Operator : JC/MD
 Sample : J6331-42
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 23 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampled :
 TP-7

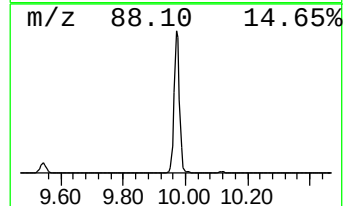
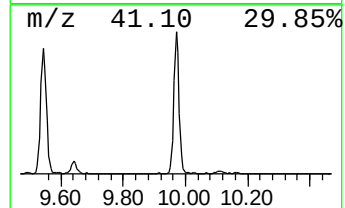
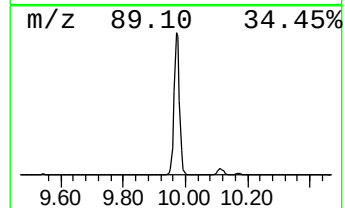
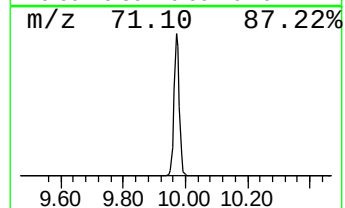
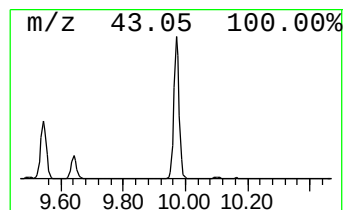
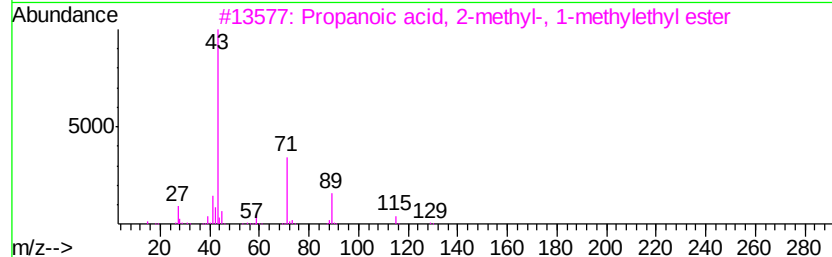
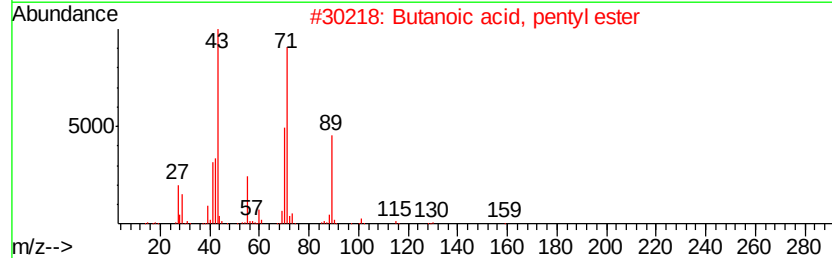
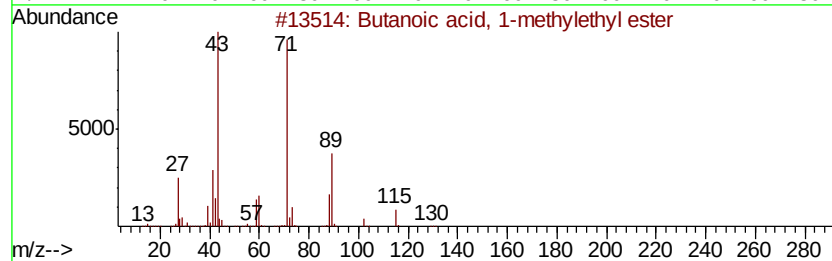
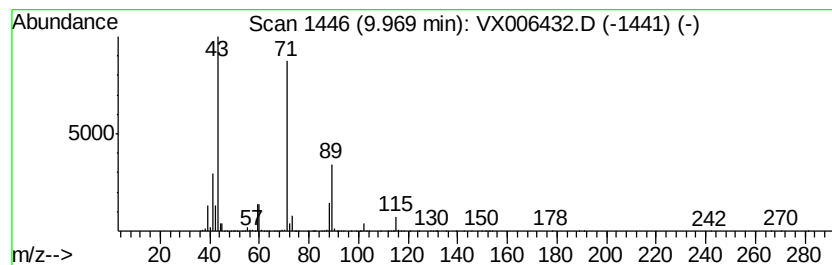
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.M
 Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	35.72 ug/l	2175810	Chlorobenzene-d5	10.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64
3		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56
4		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	56
5		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX121118\
Data File : VX006432.D
Acq On : 11 Dec 2018 20:24
Operator : JC/MD
Sample : J6331-42
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
TP-7

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X112918W.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	86.2	ug/l	4409600	2	6.86	2558330	50.0
Propanoic acid, 1...	8.62	12.9	ug/l	783917	3	10.12	3045400	50.0
Propanoic acid, 2...	9.31	7.2	ug/l	440857	3	10.12	3045400	50.0
Propanoic acid, p...	9.54	47.7	ug/l	2907760	3	10.12	3045400	50.0
Butanoic acid, 1-...	9.97	35.7	ug/l	2175810	3	10.12	3045400	50.0