

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX122718\
 Data File : VX006844.D
 Acq On : 27 Dec 2018 16:02
 Operator : JC/MD
 Sample : J6195-12
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 OR-01-122618-A

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\82X121818W.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	1.654	66	82	85	rBV4	53567	203623	4.60%	0.594%
2	2.446	207	212	219	rVB	42927	71845	1.62%	0.210%
3	2.855	272	279	293	rVV	2294890	4422731	100.00%	12.910%
4	5.507	703	714	724	rBV2	356309	1013888	22.92%	2.960%
5	5.659	729	739	753	rVV	643092	1812921	40.99%	5.292%
6	6.068	790	806	821	rBV	377777	975525	22.06%	2.848%
7	6.458	861	870	881	rBV2	24864	65407	1.48%	0.191%
8	6.860	926	936	951	rBV	934433	2221104	50.22%	6.483%
9	7.549	1044	1049	1056	rBV	22093	47903	1.08%	0.140%
10	7.878	1095	1103	1119	rBV	2449014	4234551	95.75%	12.361%
11	8.616	1216	1224	1233	rBV	495810	756658	17.11%	2.209%
12	8.713	1233	1240	1249	rVV	2018235	3151159	71.25%	9.198%
13	9.018	1285	1290	1301	rBV	53493	88287	2.00%	0.258%
14	9.305	1329	1337	1344	rBV	307182	444390	10.05%	1.297%
15	9.408	1350	1354	1357	rVV	119546	162973	3.68%	0.476%
16	9.439	1357	1359	1366	rVB	40324	50173	1.13%	0.146%
17	9.543	1370	1376	1382	rBV	2301292	2918859	66.00%	8.520%
18	9.640	1388	1392	1401	rVB	161796	216407	4.89%	0.632%
19	9.969	1440	1446	1458	rBV	1784420	2203144	49.81%	6.431%
20	10.110	1462	1469	1477	rBV	2002655	2749652	62.17%	8.026%
21	10.695	1560	1565	1574	rVB2	123498	157310	3.56%	0.459%
22	11.134	1632	1637	1648	rBV	1728384	2206100	49.88%	6.440%
23	11.506	1694	1698	1707	rVB	35191	48055	1.09%	0.140%
24	11.804	1742	1747	1752	rBV	68448	86190	1.95%	0.252%
25	12.079	1786	1792	1798	rBV	2155494	2670836	60.39%	7.796%
26	12.140	1798	1802	1810	rVB	56142	75280	1.70%	0.220%
27	12.298	1820	1828	1836	rBV2	62896	108920	2.46%	0.318%
28	12.371	1836	1840	1850	rVB2	32590	55851	1.26%	0.163%
29	12.755	1899	1903	1911	rBV2	38094	64074	1.45%	0.187%
30	13.018	1943	1946	1951	rVB	40166	48852	1.10%	0.143%
31	13.225	1976	1980	1983	rVB	45675	54761	1.24%	0.160%
32	13.347	1996	2000	2006	rVB2	122961	161519	3.65%	0.471%
33	13.481	2016	2022	2028	rVB	83042	111425	2.52%	0.325%
34	13.719	2053	2061	2066	rVB4	25278	55853	1.26%	0.163%

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Integrator: RTE
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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	13.835	2073	2080	2086	rVB	110963	148427	3.36%	0.433%
36	13.981	2098	2104	2108	rBV3	33575	49503	1.12%	0.144%
37	14.286	2147	2154	2161	rBV	69491	118080	2.67%	0.345%
38	14.536	2191	2195	2200	rVB2	41613	54936	1.24%	0.160%
39	14.694	2212	2221	2225	rBV	68967	110872	2.51%	0.324%
40	14.834	2239	2244	2250	rBV	43406	60195	1.36%	0.176%

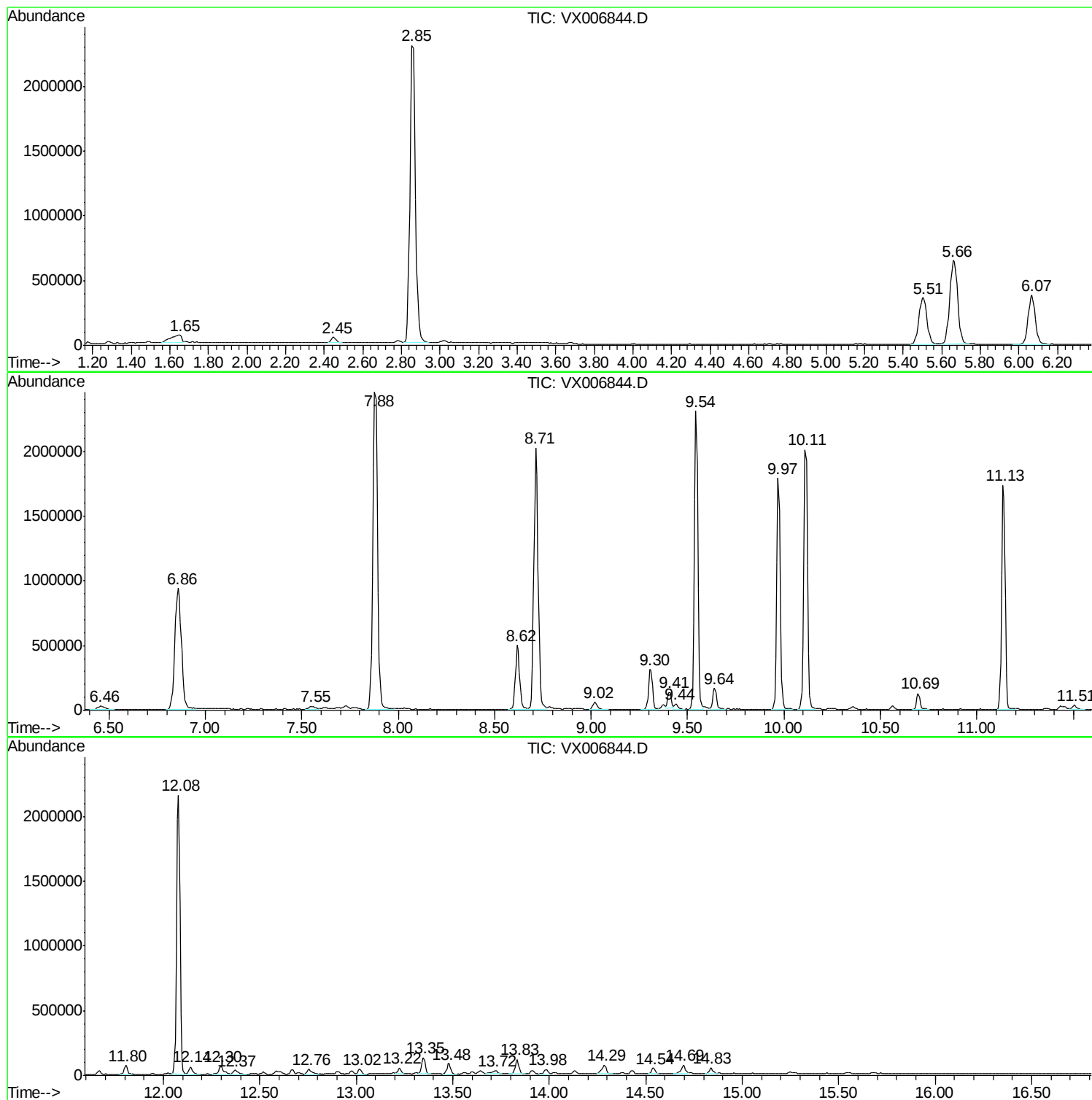
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Quant Title : SW846 8260

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



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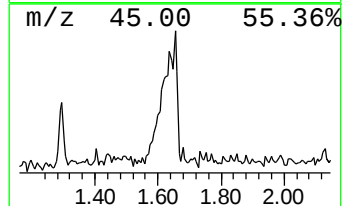
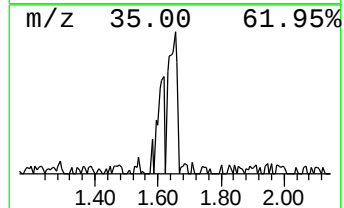
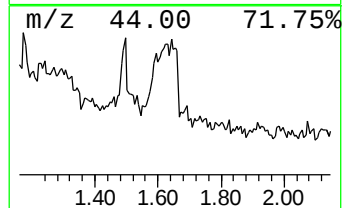
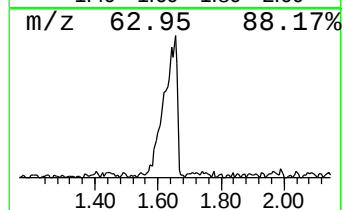
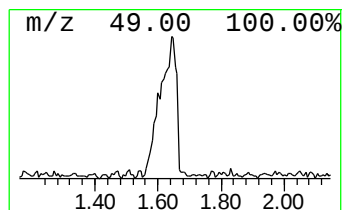
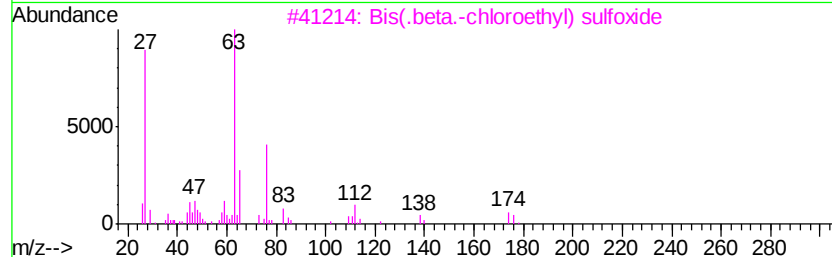
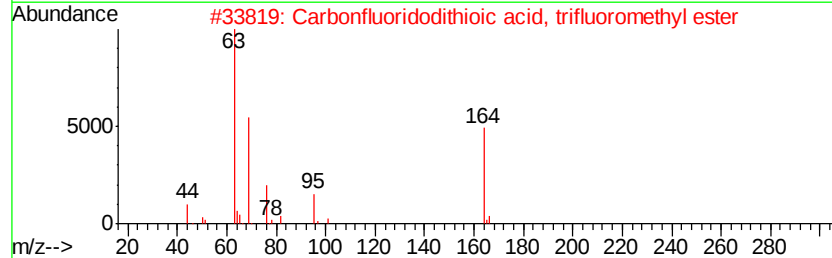
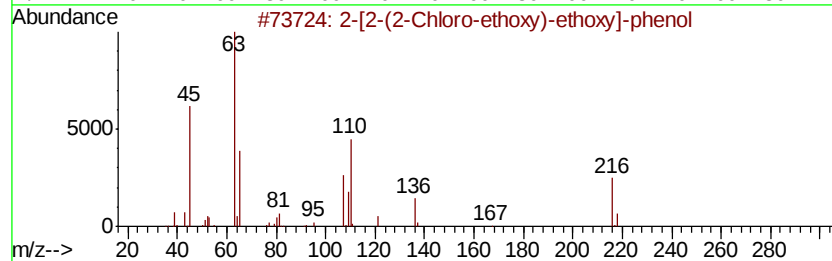
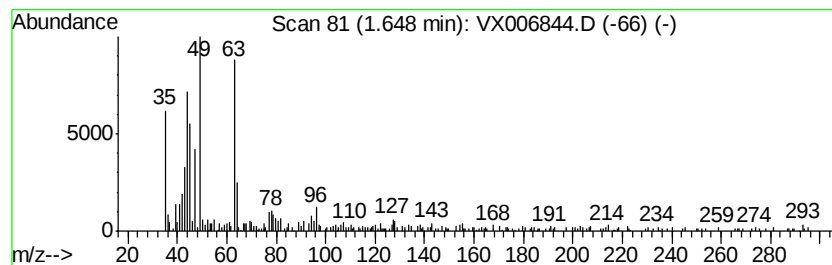
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Quant Title : SW846 8260

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

Peak Number 1 unknown1.65 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.65	5.62 ug/l	203623	Pentafluorobenzene	5.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	25
2			Carbonfluoridodithioic acid, tri...	164	C2F4S2	000371-73-3	10
3			Bis(.beta.-chloroethyl) sulfoxide	174	C4H8Cl2OS	005819-08-9	10
4			Silane, bis(fluoromethyl)dimethyl-	124	C4H10F2Si	065864-63-3	10
5			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	017639-93-9	9



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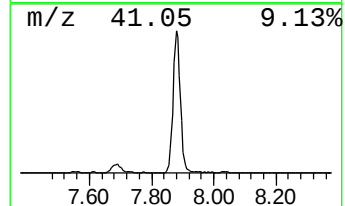
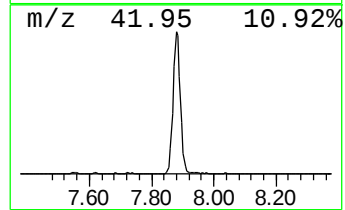
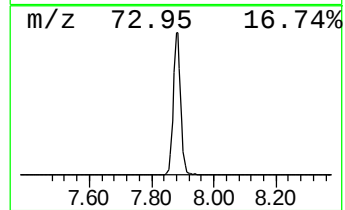
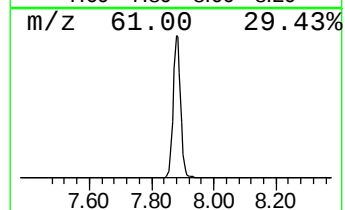
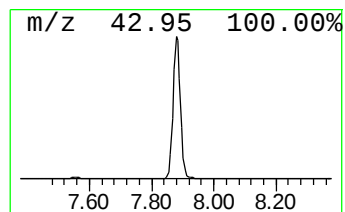
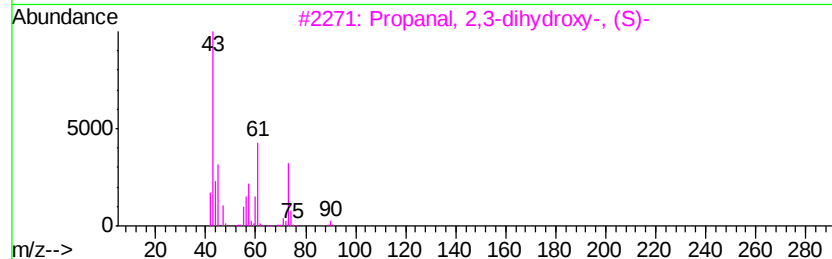
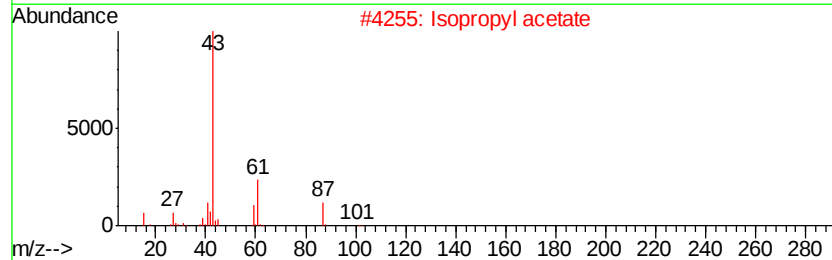
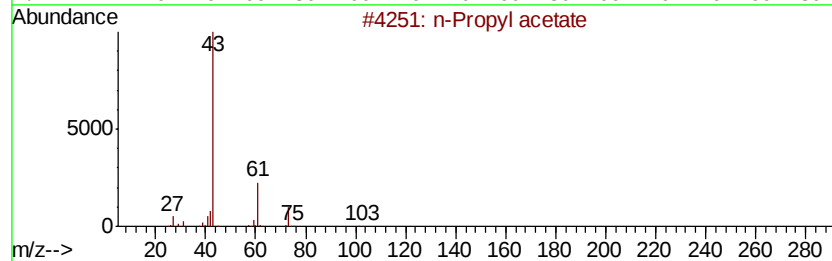
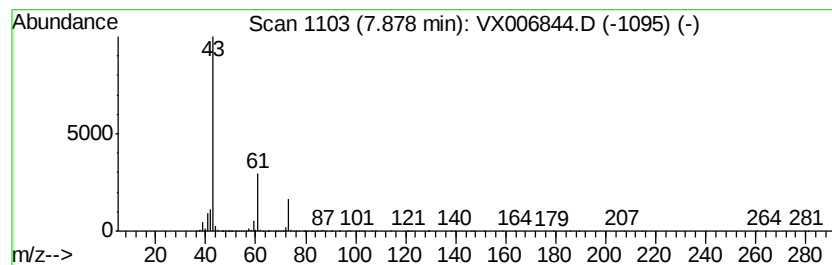
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Peak Number 2 n-Propyl acetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.88	95.33 ug/l	4234550	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	9
3		Propanal, 2,3-dihydroxy-, (S)-	90	C3H6O3	000497-09-6	9
4		1-Butanamine	73	C4H11N	000109-73-9	7
5		Isobutylamine	73	C4H11N	000078-81-9	4



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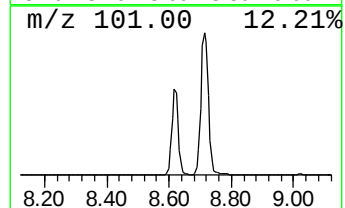
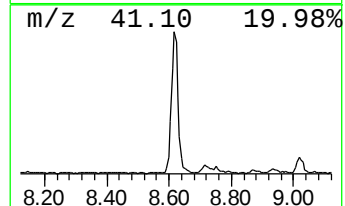
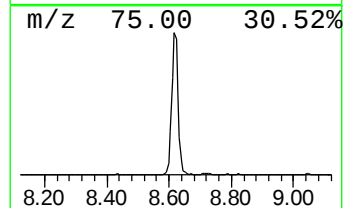
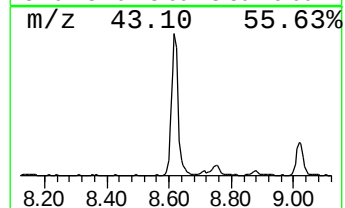
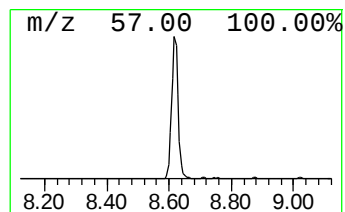
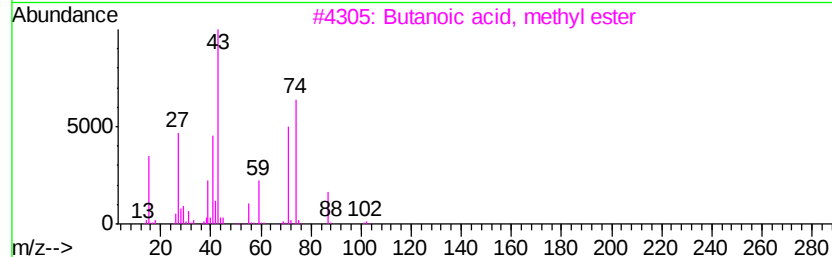
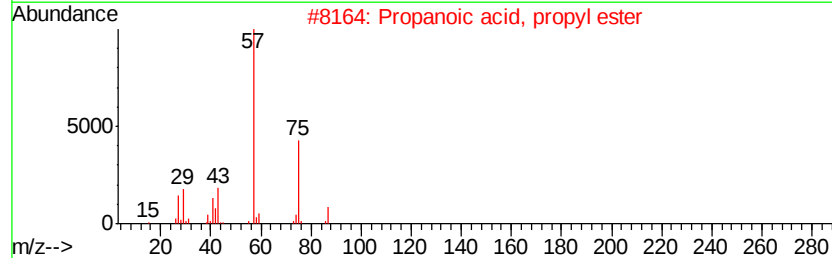
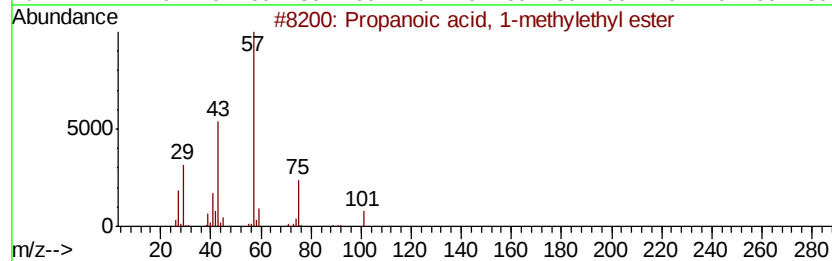
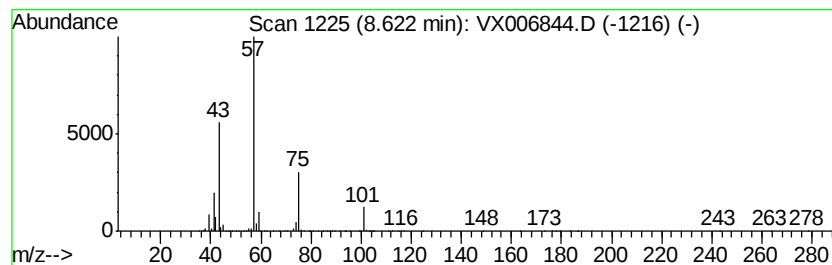
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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.62	13.76 ug/l	756658	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	50	
3	Butanoic acid, methyl ester	102	C5H10O2	000623-42-7	10	
4	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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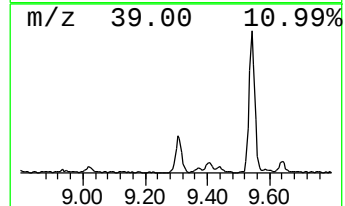
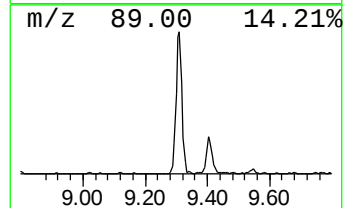
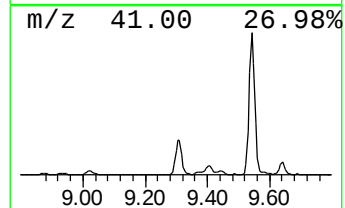
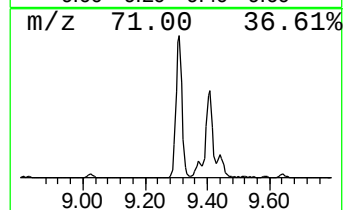
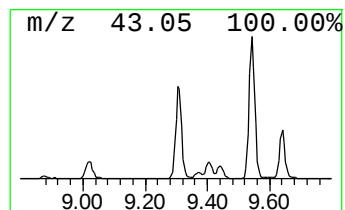
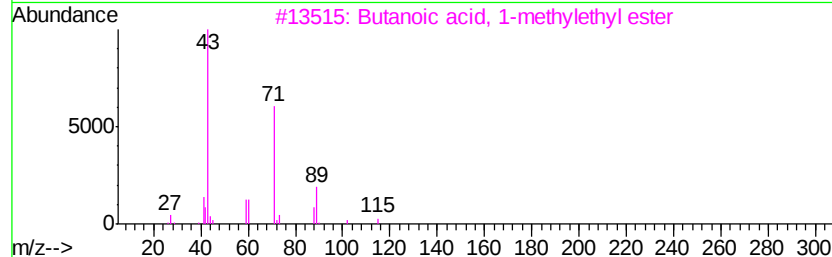
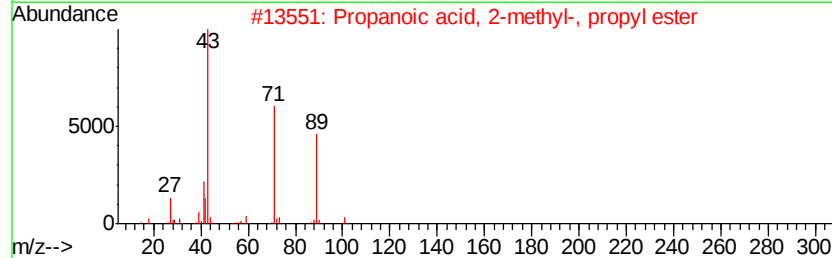
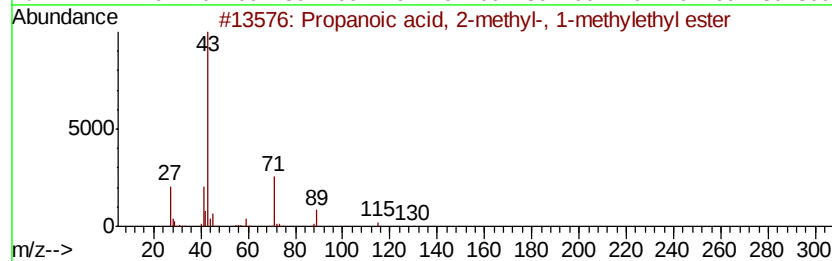
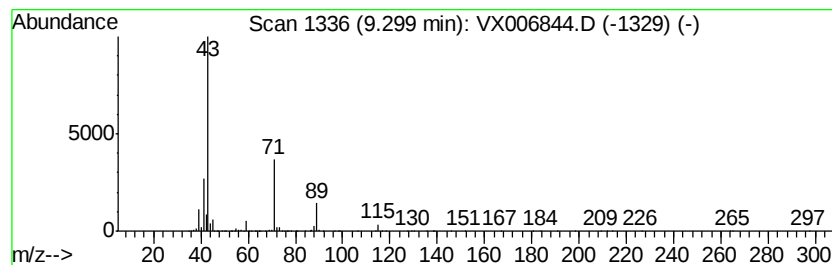
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Peak Number 4 Propanoic acid, 2-methyl-, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.30	8.08 ug/l	444390	Chlorobenzene-d5	10.11

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	72
3		Butanoic acid, 1-methyllethyl ester	130	C7H14O2	000638-11-9	56
4		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	50
5		3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	38



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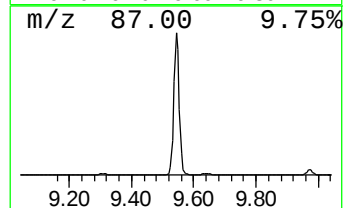
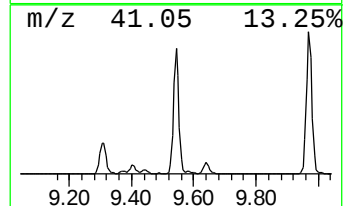
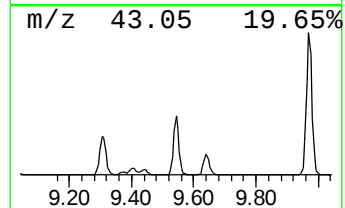
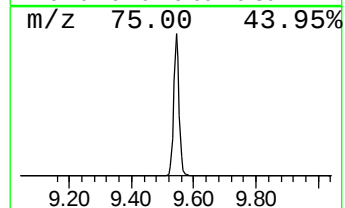
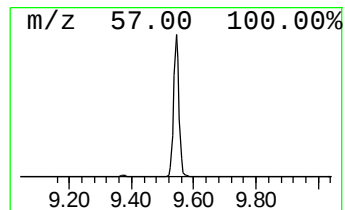
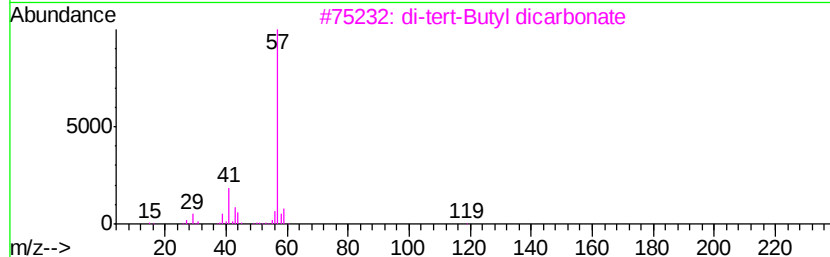
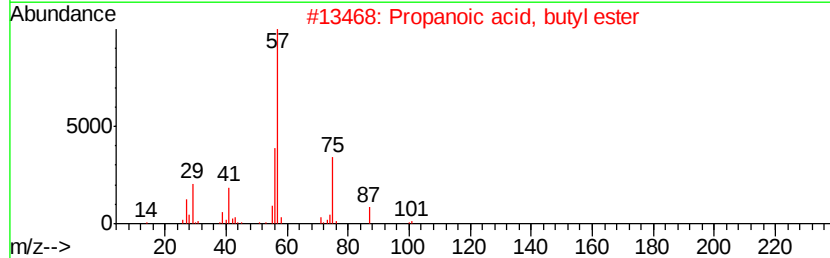
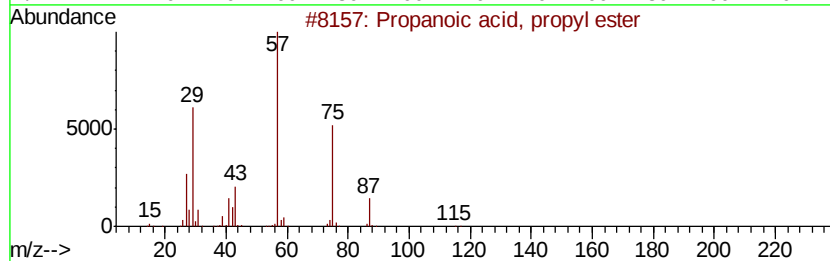
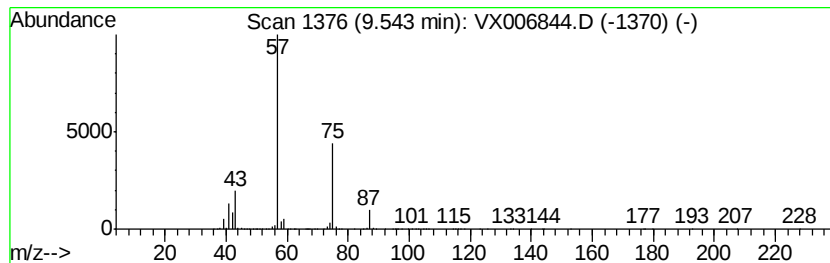
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propanoic acid, propyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.54	53.08 ug/l	2918860	Chlorobenzene-d5	10.11

Hit# of	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, propyl ester	116	C6H12O2	000106-36-5	83
2	Propanoic acid, butyl ester	130	C7H14O2	000590-01-2	40
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	9
4	Acetaldehyde, O-ethyloxime-	87	C4H9NO	1000288-34-6	7
5	1-Butanamine, 2-methyl-	87	C5H13N	000096-15-1	7



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX122718\
Data File : VX006844.D
Acq On : 27 Dec 2018 16:02
Operator : JC/MD
Sample : J6195-12
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
OR-01-122618-A

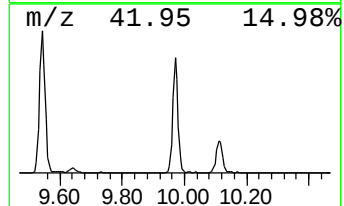
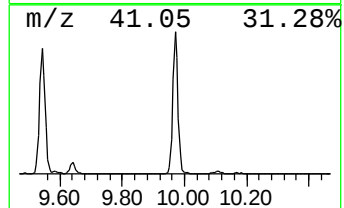
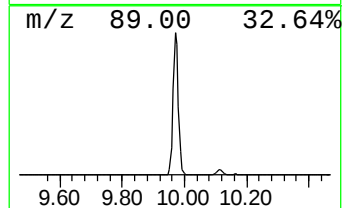
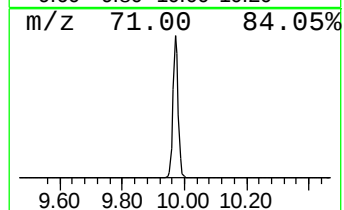
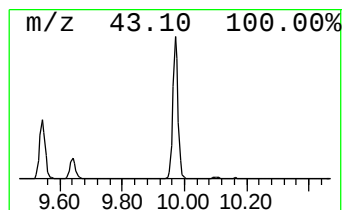
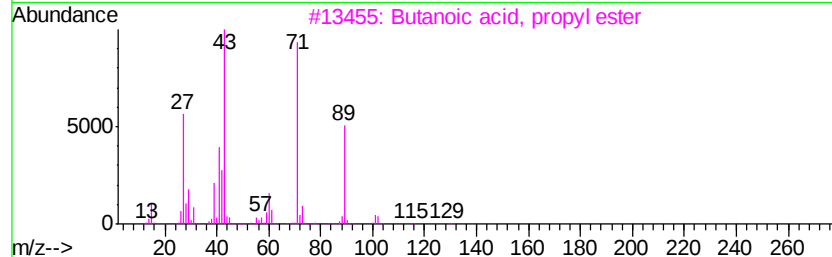
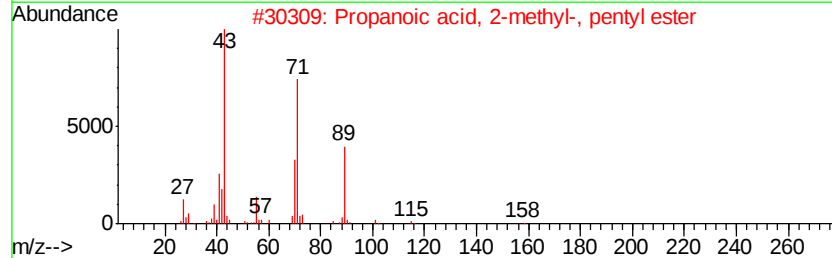
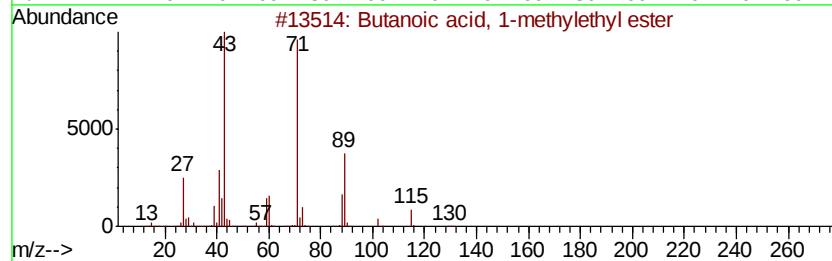
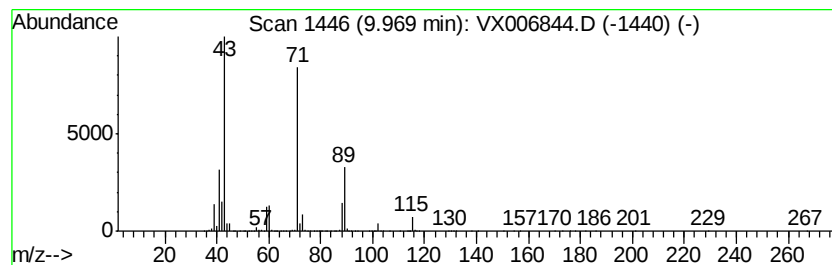
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.M
Quant Title : SW846 8260

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

Peak Number 6 Butanoic acid, 1-methylethy... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.97	40.06 ug/l	2203140	Chlorobenzene-d5	10.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	91
2		Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64
3		Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	59
4		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	56
5		Propanoic acid, 2-methyl-, 1-met...	130	C7H14O2	000617-50-5	56



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX122718\
Data File : VX006844.D
Acq On : 27 Dec 2018 16:02
Operator : JC/MD
Sample : J6195-12
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
OR-01-122618-A

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X121818W.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
unknown1.65	1.65	5.6	ug/l	203623	1	5.67	1812920	50.0
n-Propyl acetate	7.88	95.3	ug/l	4234550	2	6.86	2221100	50.0
Propanoic acid, 1...	8.62	13.8	ug/l	756658	3	10.11	2749650	50.0
Propanoic acid, 2...	9.30	8.1	ug/l	444390	3	10.11	2749650	50.0
Propanoic acid, p...	9.54	53.1	ug/l	2918860	3	10.11	2749650	50.0
Butanoic acid, 1-...	9.97	40.1	ug/l	2203140	3	10.11	2749650	50.0