

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX100518\
 Data File : VX005074.D
 Acq On : 05 Oct 2018 18:51
 Operator : JC/MD
 Sample : J5188-08
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 NS-092818

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\82X092618W.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	1.489	51	55	62	rVB	20427	25725	1.92%	0.250%
2	1.611	68	75	78	rVB4	8048	15995	1.19%	0.156%
3	2.446	206	212	220	rVB	29906	48931	3.65%	0.476%
4	2.855	273	279	287	rVB	37918	68034	5.08%	0.662%
5	3.672	407	413	423	rVB3	10920	30990	2.31%	0.302%
6	4.775	588	594	610	rVB2	6343	21155	1.58%	0.206%
7	5.214	650	666	679	rVB4	9035	32305	2.41%	0.314%
8	5.501	700	713	727	rBV	163037	468179	34.93%	4.556%
9	5.665	727	740	760	rBV	210576	614896	45.87%	5.984%
10	6.068	796	806	826	rVB2	181153	474305	35.39%	4.616%
11	6.464	861	871	890	rBV	140529	368522	27.49%	3.587%
12	6.860	924	936	963	rBV	340658	854818	63.77%	8.319%
13	7.683	1063	1071	1076	rBV3	7790	19857	1.48%	0.193%
14	7.884	1097	1104	1119	rBV	209599	376237	28.07%	3.662%
15	8.720	1233	1241	1249	rBV	790515	1340386	100.00%	13.045%
16	9.409	1350	1354	1358	rVB	18058	21818	1.63%	0.212%
17	9.549	1371	1377	1381	rBV	91270	124901	9.32%	1.216%
18	9.585	1381	1383	1389	rVV3	11376	21100	1.57%	0.205%
19	9.640	1389	1392	1403	rVB	33279	46657	3.48%	0.454%
20	9.976	1440	1447	1459	rBV	91941	126634	9.45%	1.232%
21	10.116	1463	1470	1489	rVV	753719	1071014	79.90%	10.423%
22	11.140	1632	1638	1654	rBV	773768	986703	73.61%	9.603%
23	11.811	1743	1748	1752	rBV	16036	21190	1.58%	0.206%
24	12.079	1786	1792	1799	rBV	992486	1205070	89.90%	11.728%
25	12.274	1819	1824	1836	rBV	131131	219875	16.40%	2.140%
26	12.371	1837	1840	1848	rVB4	8667	18929	1.41%	0.184%
27	13.347	1993	2000	2005	rVB3	16243	26097	1.95%	0.254%
28	13.481	2015	2022	2029	rBV2	31172	59249	4.42%	0.577%
29	13.646	2045	2049	2052	rBV5	9968	14501	1.08%	0.141%
30	13.688	2052	2056	2060	rVV5	9380	20008	1.49%	0.195%
31	13.835	2075	2080	2085	rVB	233201	284205	21.20%	2.766%
32	13.981	2098	2104	2109	rVB6	12561	28326	2.11%	0.276%
33	14.133	2125	2129	2133	rVB	15187	17292	1.29%	0.168%
34	14.280	2145	2153	2163	rVB3	20450	49350	3.68%	0.480%

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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 >
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35	14.377	2165	2169	2174	rVB	17917	21774	1.62%	0.212%
36	14.432	2174	2178	2183	rVB	14431	18745	1.40%	0.182%
37	14.542	2192	2196	2207	rVB2	21839	35780	2.67%	0.348%
38	14.694	2211	2221	2231	rBV	287917	423412	31.59%	4.121%
39	14.840	2238	2245	2254	rVB	226791	281825	21.03%	2.743%
40	14.975	2263	2267	2273	rBV3	19774	35018	2.61%	0.341%
41	15.060	2277	2281	2284	rVB4	15412	23057	1.72%	0.224%
42	15.273	2313	2316	2320	rVB	16684	23160	1.73%	0.225%
43	15.444	2340	2344	2347	rBV3	11077	16541	1.23%	0.161%
44	15.554	2357	2362	2374	rVB3	29703	58672	4.38%	0.571%
45	15.688	2374	2384	2388	rVV	44130	86330	6.44%	0.840%
46	15.724	2388	2390	2398	rVB	22623	32445	2.42%	0.316%
47	15.920	2413	2422	2428	rBV5	12750	36800	2.75%	0.358%
48	16.072	2441	2447	2451	rBV2	10472	20488	1.53%	0.199%
49	16.170	2458	2463	2469	rVB6	11763	22501	1.68%	0.219%
50	16.419	2499	2504	2508	rBV2	8178	15297	1.14%	0.149%

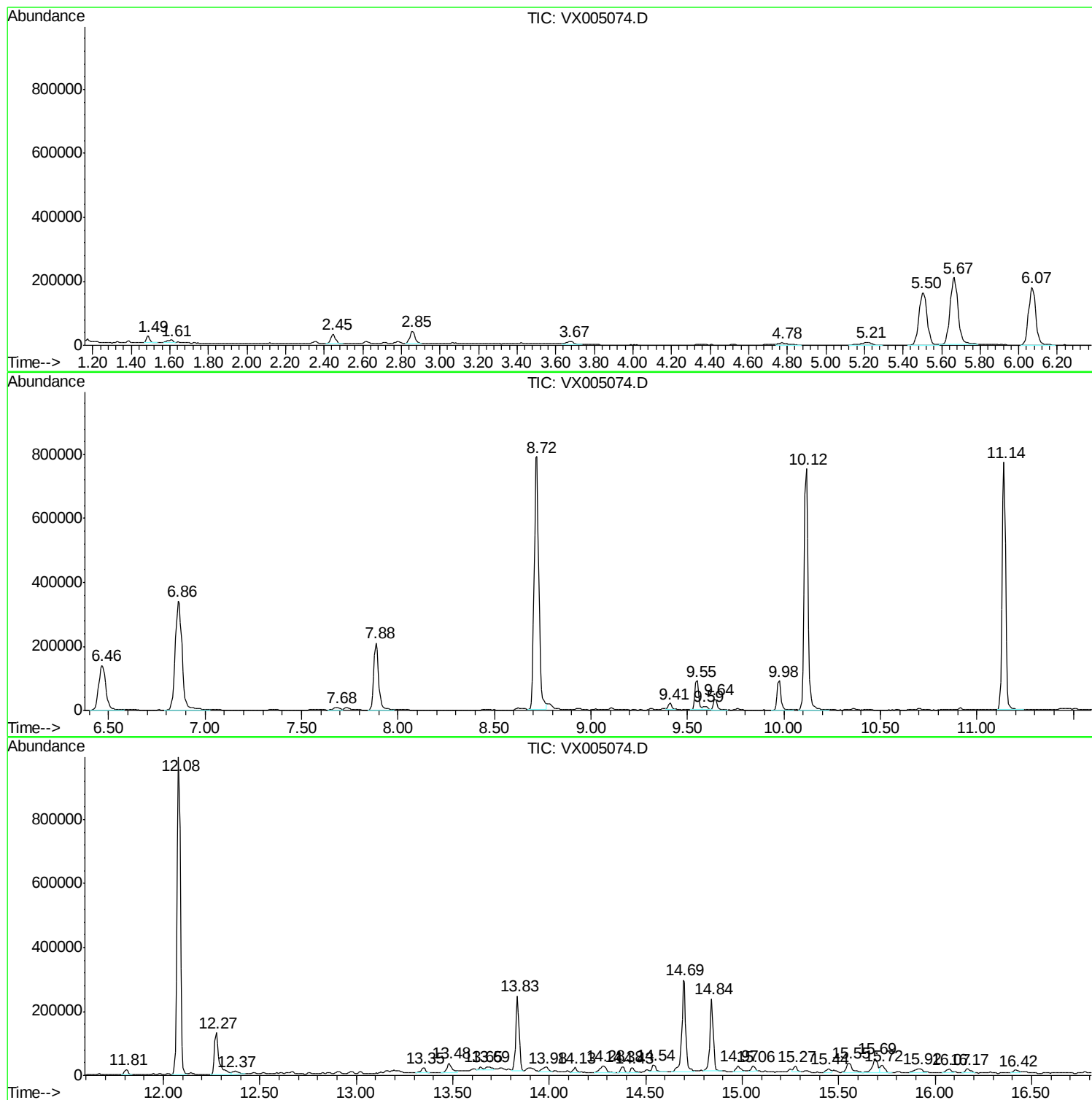
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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



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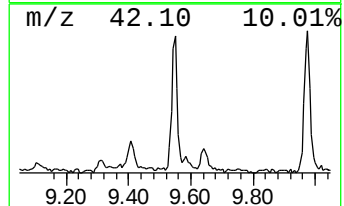
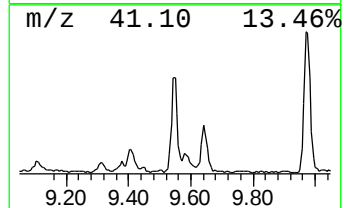
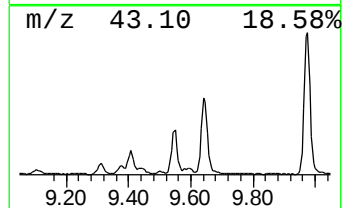
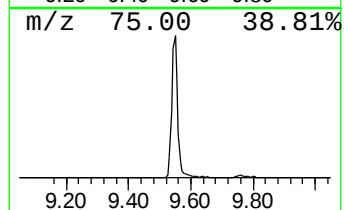
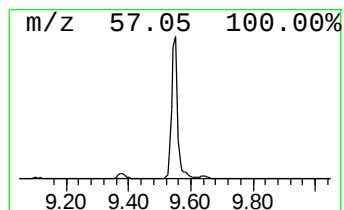
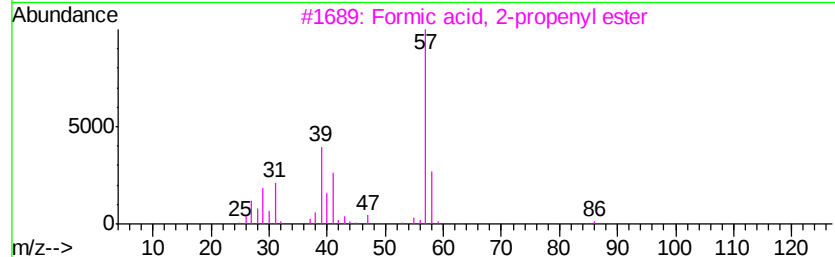
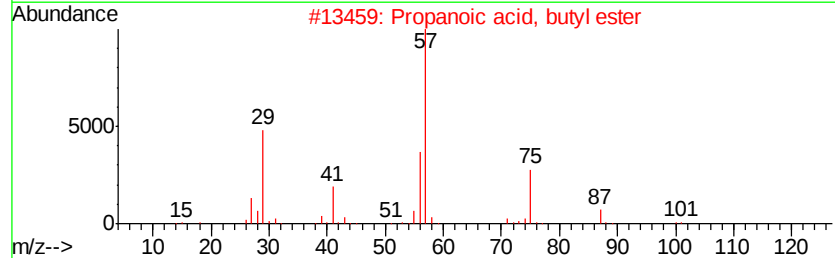
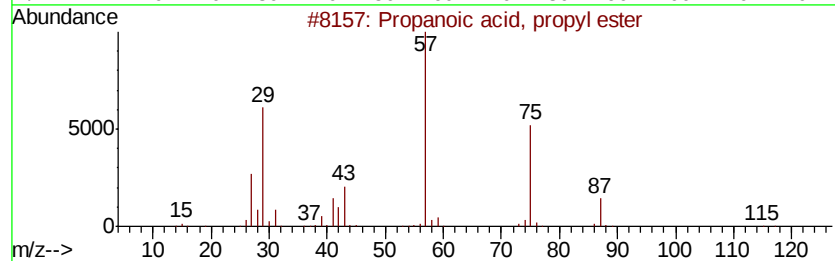
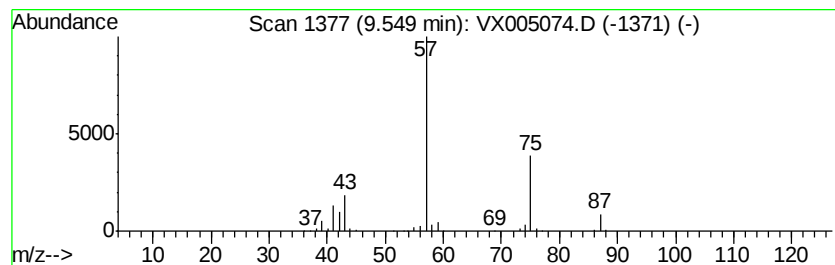
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 1 Propanoic acid, propyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	5.83 ug/l	124901	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	45
3		Formic acid, 2-propenyl ester	86	C4H6O2	001838-59-1	7
4		1-Butanamine, 3-methyl-	87	C5H13N	000107-85-7	7
5		1-Penten-3-ol	86	C5H10O	000616-25-1	4



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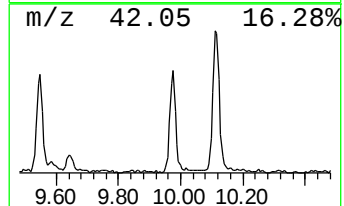
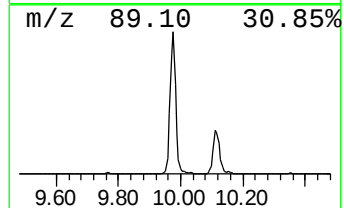
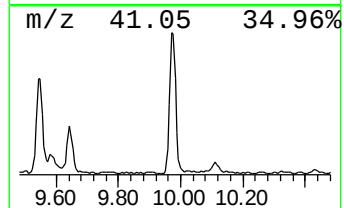
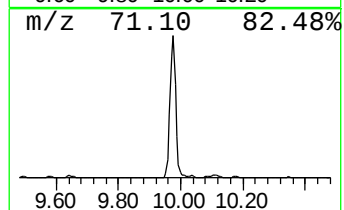
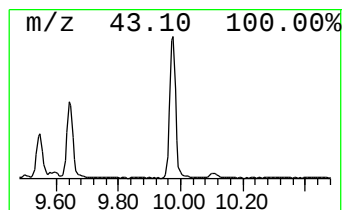
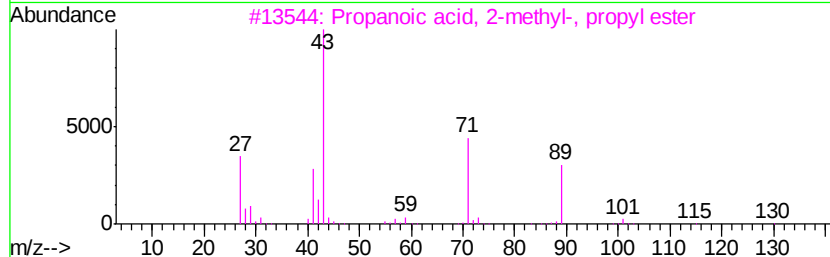
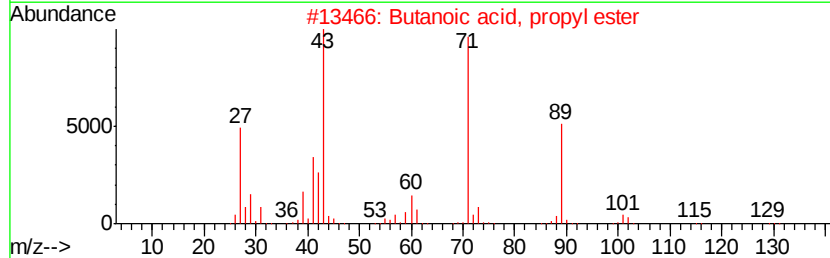
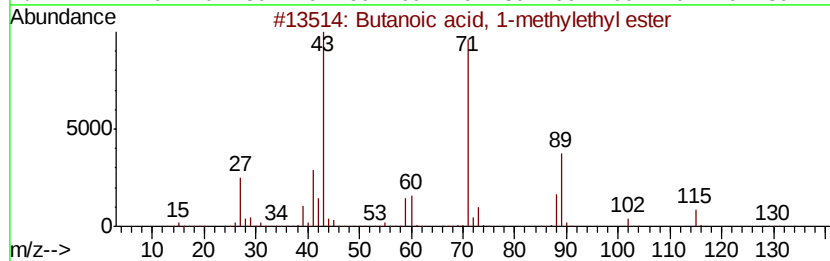
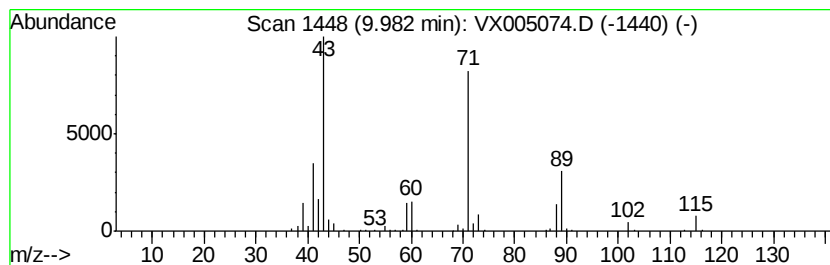
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 Butanoic acid, 1-methylethy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.98	5.91 ug/l	126634	Chlorobenzene-d5	10.12

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanoic acid, 1-methylethyl ester	130	C7H14O2	000638-11-9	90
2			Butanoic acid, propyl ester	130	C7H14O2	000105-66-8	72
3			Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	72
4			Propanoic acid, 2-methyl-, pentyl...	158	C9H18O2	002445-72-9	64
5			Butanoic acid, pentyl ester	158	C9H18O2	000540-18-1	64



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 7 Sample Multiplier: 1

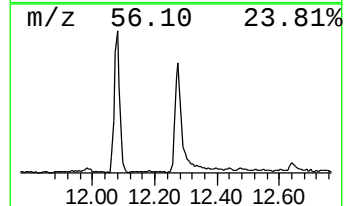
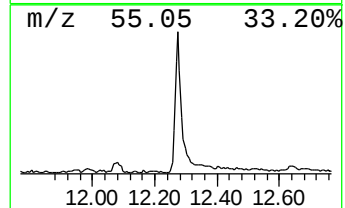
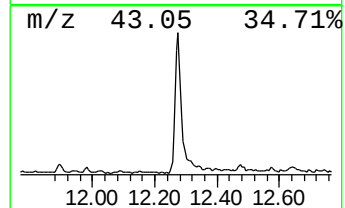
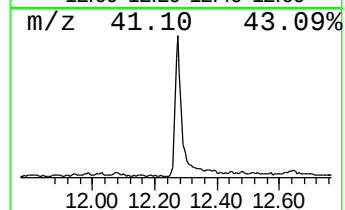
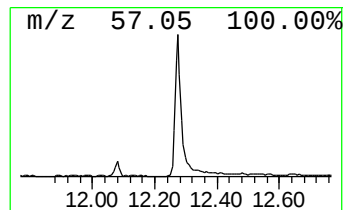
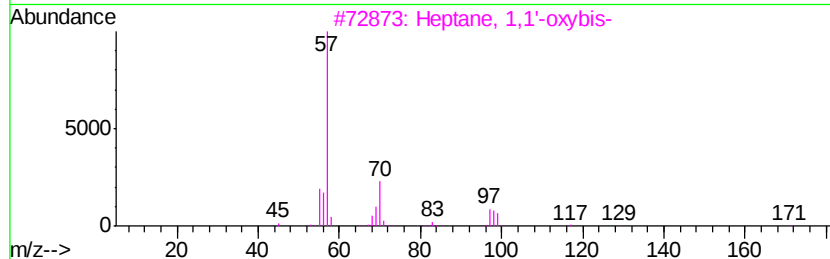
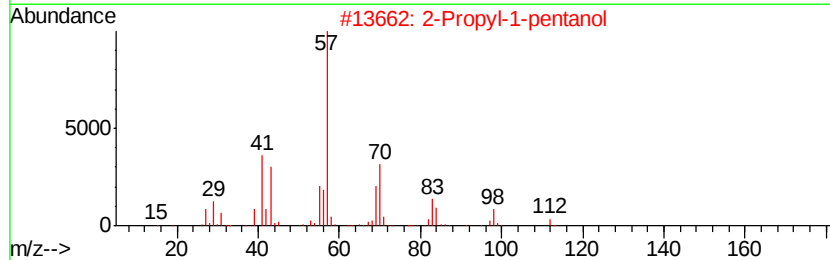
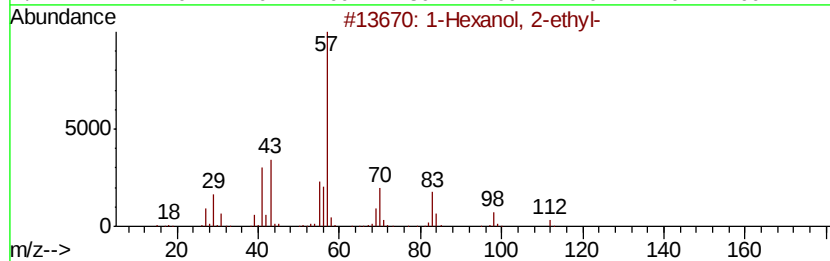
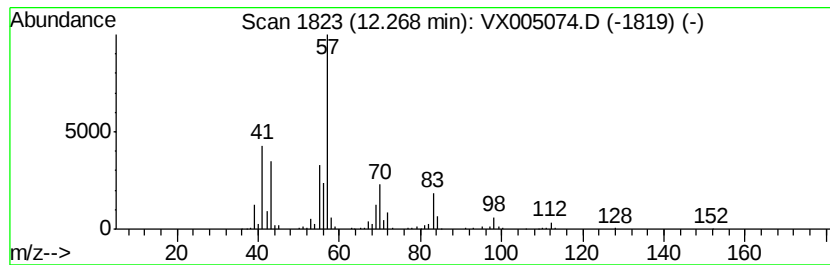
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.27	9.12 ug/l	219875	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Hexanol, 2-ethyl-	130 C8H18O	000104-76-7	86
2	2-Propyl-1-pentanol	130 C8H18O	058175-57-8	50
3	Heptane, 1,1'-oxybis-	214 C14H30O	000629-64-1	50
4	Octane, 2,3-dimethyl-	142 C10H22	007146-60-3	40
5	1-Pentanol, 2-ethyl-4-methyl-	130 C8H18O	000106-67-2	38



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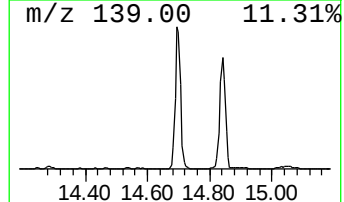
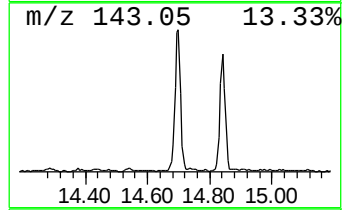
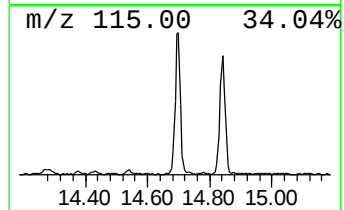
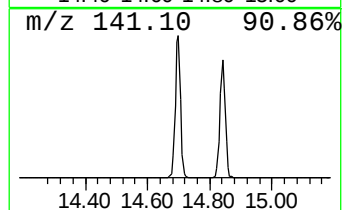
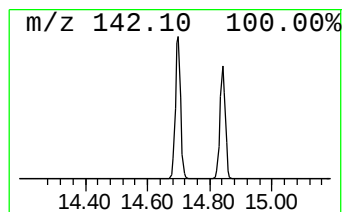
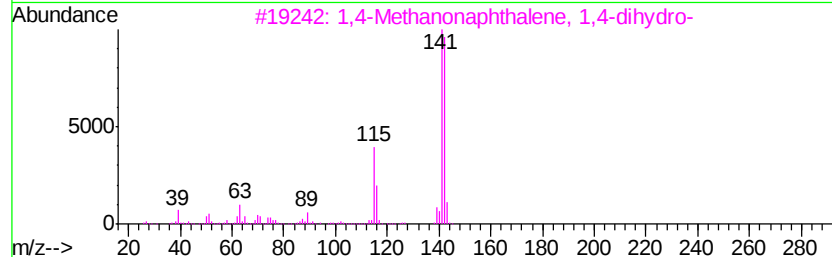
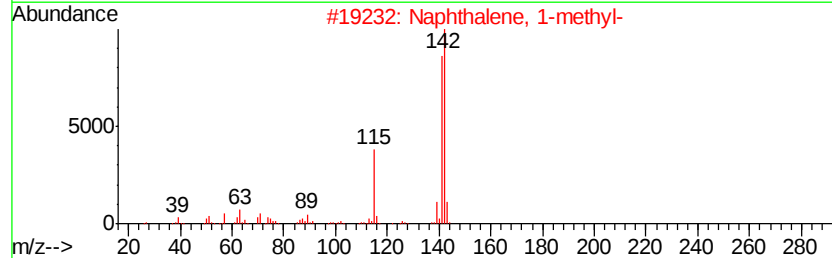
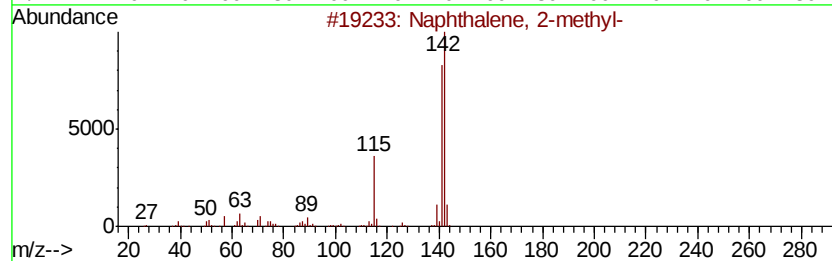
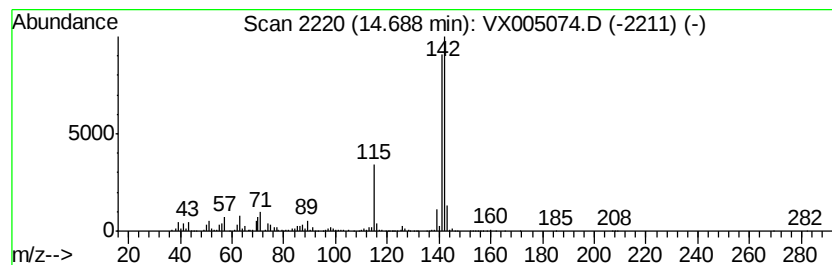
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Naphthalene, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	17.57 ug/l	423412	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2		Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	90
4		Benzocycloheptatriene	142	C11H10	000264-09-5	90
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



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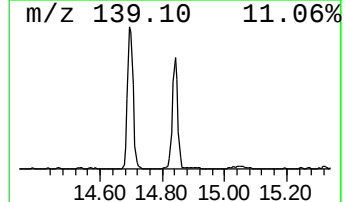
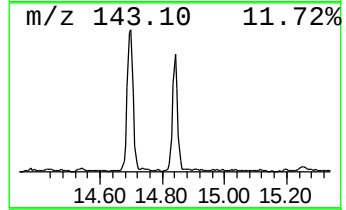
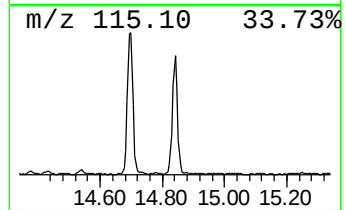
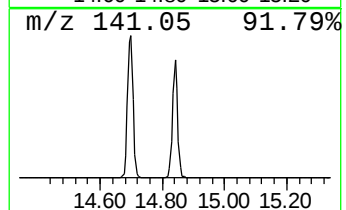
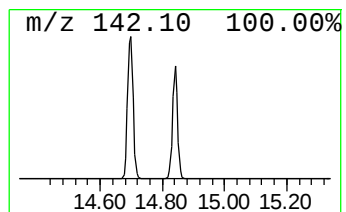
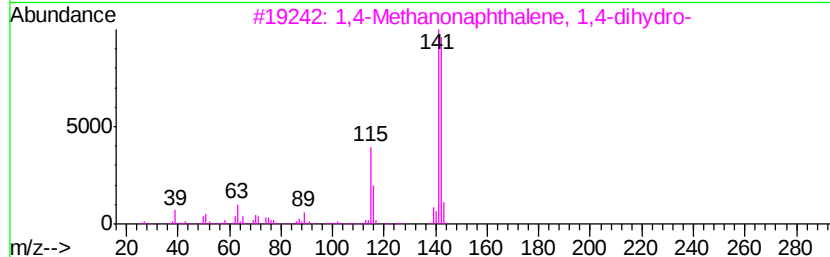
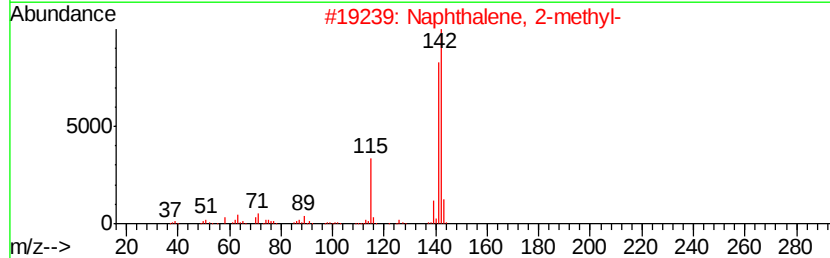
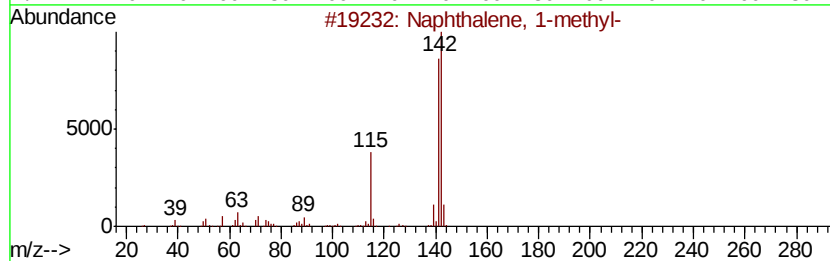
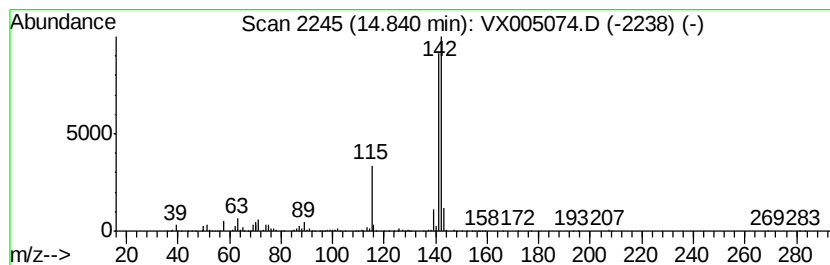
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.M
Quant Title : SW846 8260

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

Peak Number 5 Naphthalene, 1-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.84	11.69 ug/l	281825	1,4-Dichlorobenzene-d4	12.08

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2		Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3		1,4-Methanonaphthalene, 1,4-dihv...	142	C11H10	004453-90-1	91
4		Benzocycloheptatriene	142	C11H10	000264-09-5	91
5		1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX100518\
Data File : VX005074.D
Acq On : 05 Oct 2018 18:51
Operator : JC/MD
Sample : J5188-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
NS-092818

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X092618W.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
Propanoic acid, p...	9.55	5.8	ug/l	124901	3	10.12	1071010	50.0
Butanoic acid, 1-...	9.98	5.9	ug/l	126634	3	10.12	1071010	50.0
1-Hexanol, 2-ethyl-	12.27	9.1	ug/l	219875	4	12.08	1205070	50.0
Naphthalene, 2-me...	14.69	17.6	ug/l	423412	4	12.08	1205070	50.0
Naphthalene, 1-me...	14.84	11.7	ug/l	281825	4	12.08	1205070	50.0