

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101918\
 Data File : VX005462.D
 Acq On : 19 Oct 2018 17:00
 Operator : JC/MD
 Sample : J5604-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MS-VB-29736-BOX-2

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\82X101218W.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	2.446	205	212	223	rBV	358091	589613	33.04%	5.463%
2	2.617	233	240	251	rBV	101454	187439	10.50%	1.737%
3	4.348	511	524	534	rBV3	13891	40441	2.27%	0.375%
4	4.708	574	583	588	rBV	10090	28656	1.61%	0.265%
5	4.763	589	592	606	rVB	7063	20714	1.16%	0.192%
6	5.159	639	657	674	rBV7	10819	53975	3.02%	0.500%
7	5.501	702	713	728	rBV	138538	398455	22.33%	3.692%
8	5.665	728	740	756	rBV	240979	686443	38.46%	6.360%
9	6.074	797	807	818	rBV	163571	414257	23.21%	3.838%
10	6.860	926	936	953	rBV	337655	835019	46.79%	7.736%
11	7.067	963	970	980	rVB2	13920	30589	1.71%	0.283%
12	7.323	1005	1012	1031	rBV	166148	357239	20.02%	3.310%
13	8.134	1135	1145	1155	rBV	30845	56551	3.17%	0.524%
14	8.713	1234	1240	1249	rBV	673098	1121514	62.84%	10.390%
15	8.787	1249	1252	1260	rVB	25016	42827	2.40%	0.397%
16	10.116	1461	1470	1482	rBV	682203	957622	53.66%	8.872%
17	10.329	1499	1505	1508	rBV	14420	23268	1.30%	0.216%
18	11.048	1618	1623	1633	rBV	1300492	1784771	100.00%	16.535%
19	11.140	1633	1638	1651	rVB	634380	859250	48.14%	7.961%
20	11.945	1765	1770	1775	rBV2	12597	22332	1.25%	0.207%
21	12.079	1787	1792	1797	rBV	788258	953295	53.41%	8.832%
22	12.274	1819	1824	1835	rBV	58846	104046	5.83%	0.964%
23	12.365	1835	1839	1845	rVB6	9404	19370	1.09%	0.179%
24	13.347	1993	2000	2006	rVB4	17783	33425	1.87%	0.310%
25	13.517	2024	2028	2033	rVB2	20791	31030	1.74%	0.287%
26	13.645	2045	2049	2055	rVB6	12190	20398	1.14%	0.189%
27	13.725	2055	2062	2069	rVB6	15123	36084	2.02%	0.334%
28	13.804	2069	2075	2089	rBV	475519	726349	40.70%	6.729%
29	13.987	2100	2105	2109	rVB2	12885	20509	1.15%	0.190%
30	14.286	2148	2154	2163	rVB3	24492	50392	2.82%	0.467%
31	14.542	2190	2196	2199	rBV3	20593	33338	1.87%	0.309%
32	14.676	2214	2218	2220	rBV2	14279	19300	1.08%	0.179%
33	14.840	2242	2245	2249	rBV2	15504	19722	1.11%	0.183%
34	15.249	2307	2312	2315	rBV3	16809	27400	1.54%	0.254%

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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

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35	15.316	2319	2323	2332	rBV	76373	125180	7.01%	1.160%
36	15.554	2357	2362	2366	rBV4	12658	19601	1.10%	0.182%
37	15.688	2380	2384	2388	rBV	15360	23864	1.34%	0.221%
38	16.419	2499	2504	2512	rVB4	7654	19382	1.09%	0.180%

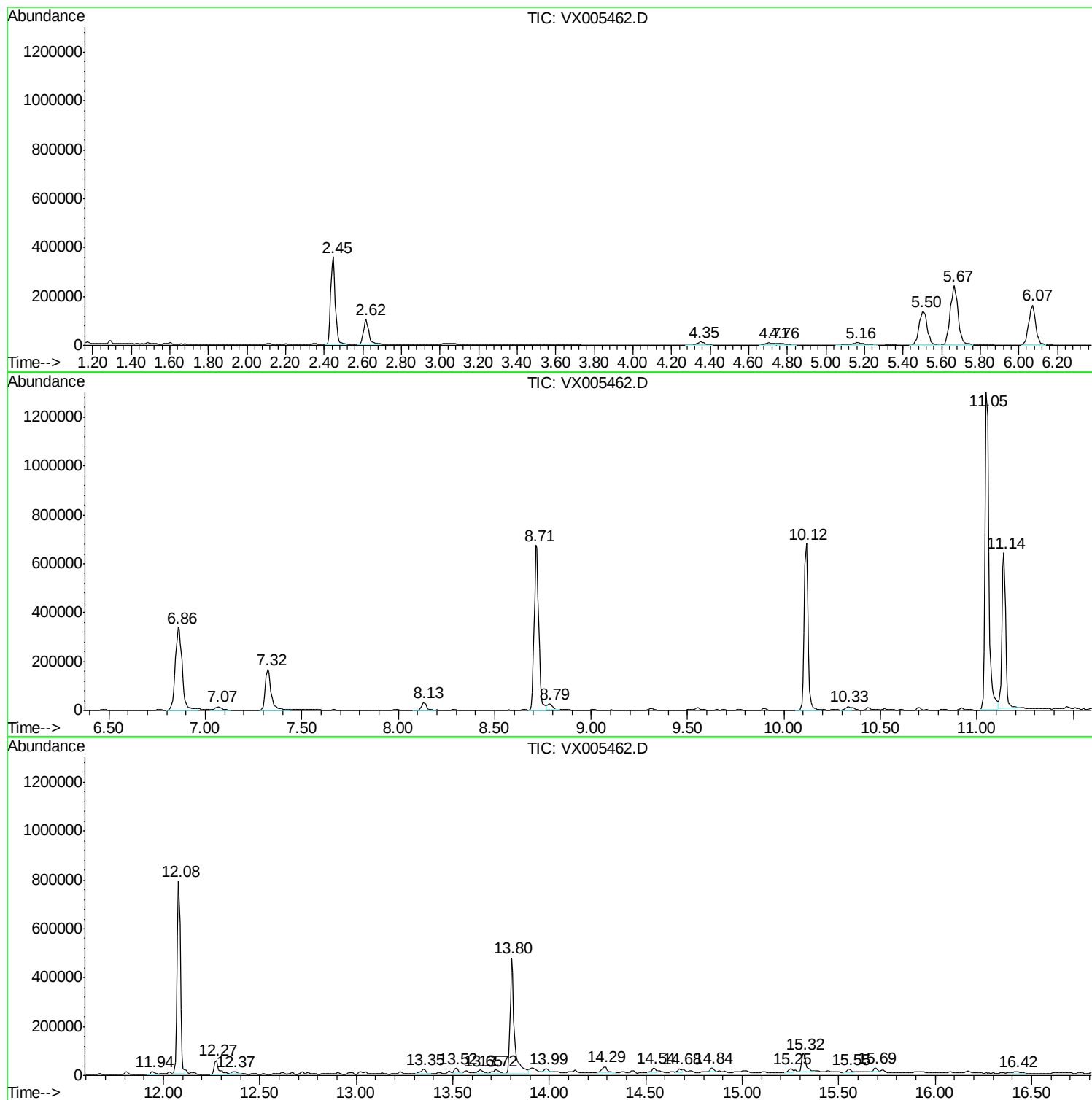
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Quant Title : SW846 8260

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



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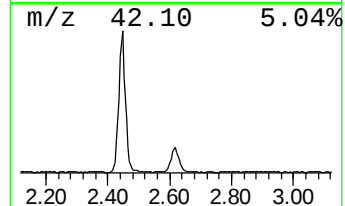
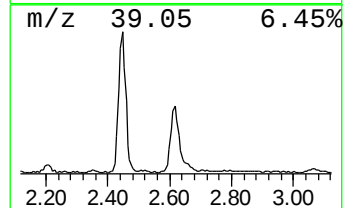
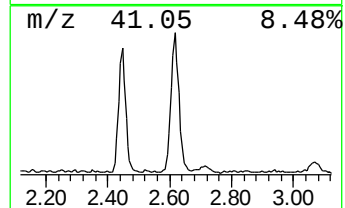
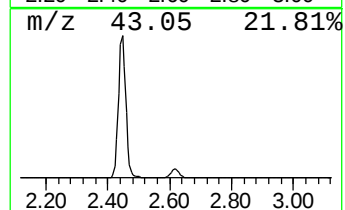
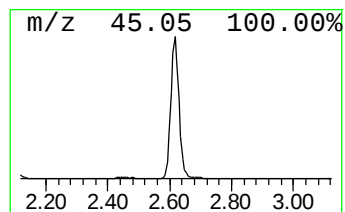
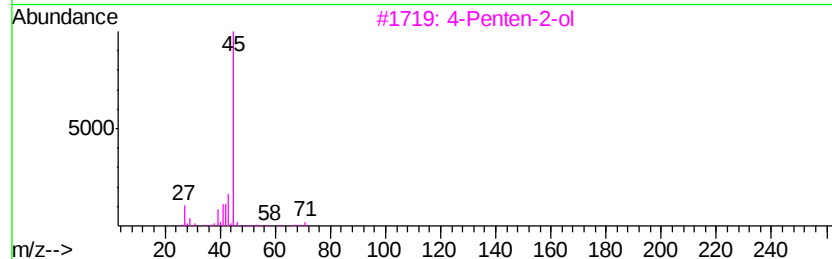
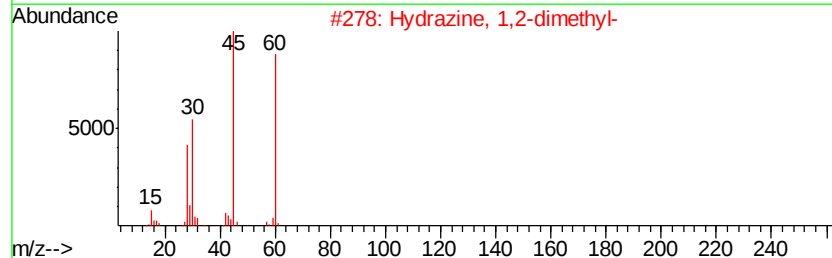
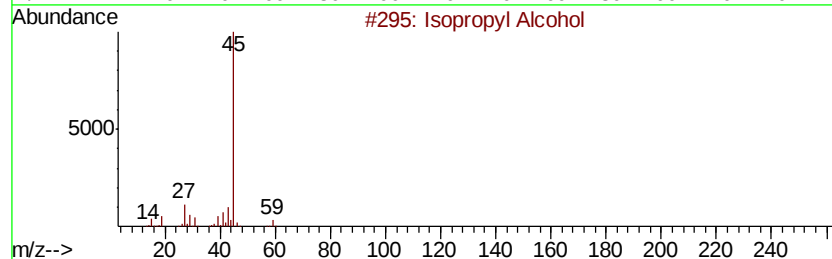
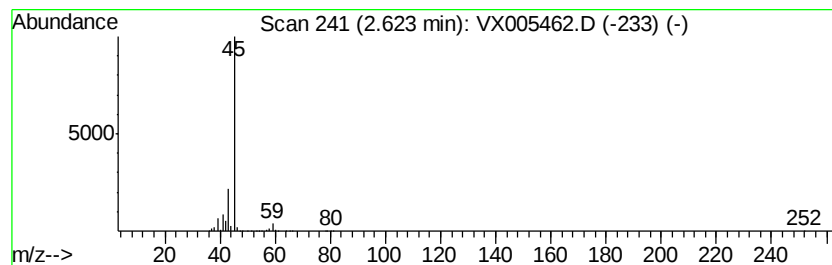
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Quant Title : SW846 8260

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

Peak Number 1 Isopropyl Alcohol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.62	13.65 ug/l	187439	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Isopropyl Alcohol	60	C3H8O	000067-63-0	90
2		Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3		4-Penten-2-ol	86	C5H10O	000625-31-0	9
4		Formamide	45	CH3NO	000075-12-7	4
5		1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4



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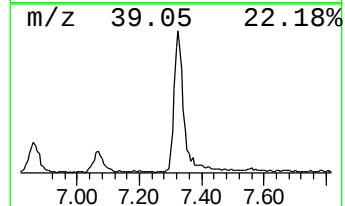
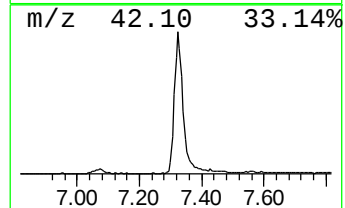
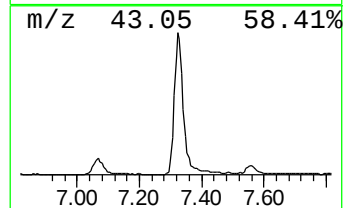
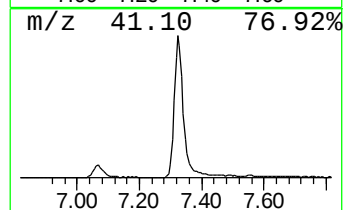
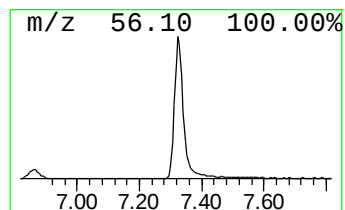
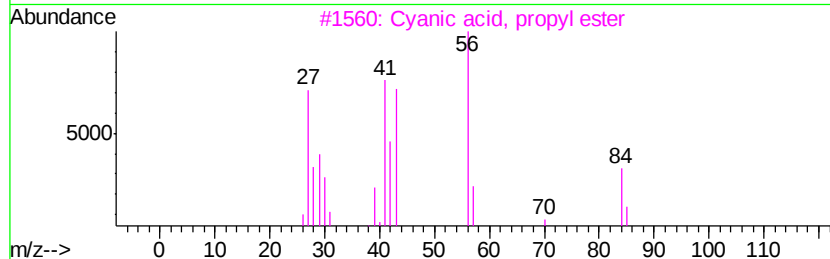
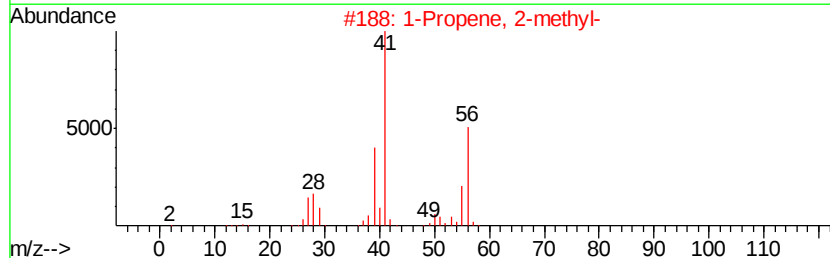
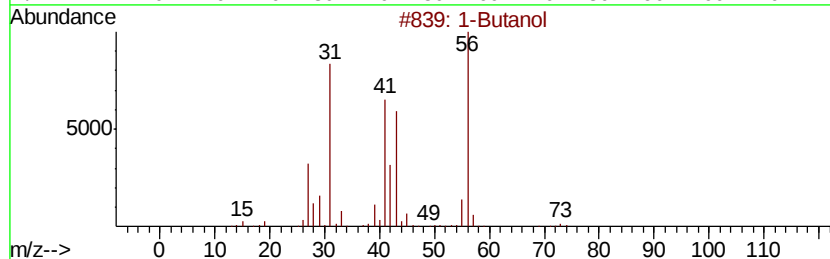
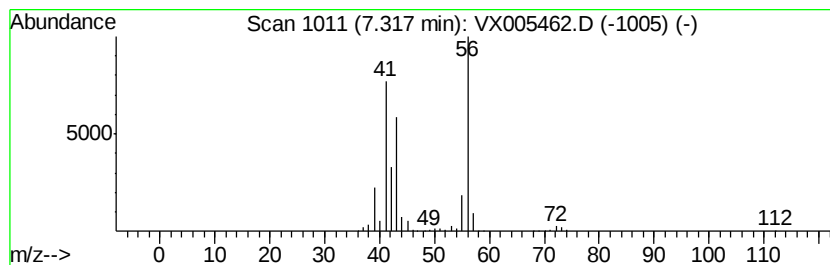
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 1-Butanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.32	21.39 ug/l	357239	1,4-Difluorobenzene	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol	74	C4H10O	000071-36-3	90
2			1-Propene, 2-methyl-	56	C4H8	000115-11-7	59
3			Cyanic acid, propyl ester	85	C4H7NO	001768-36-1	50
4			3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	45
5			1-Hexanol	102	C6H14O	000111-27-3	38



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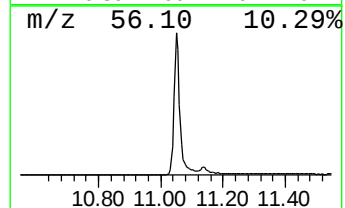
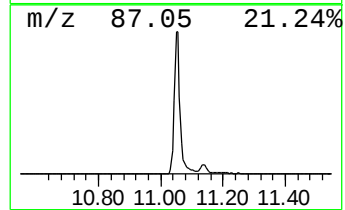
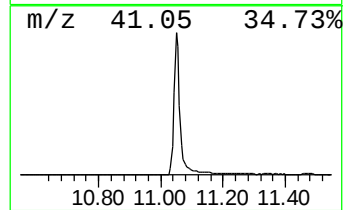
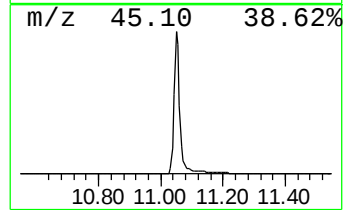
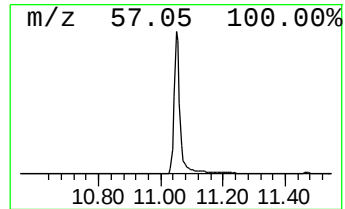
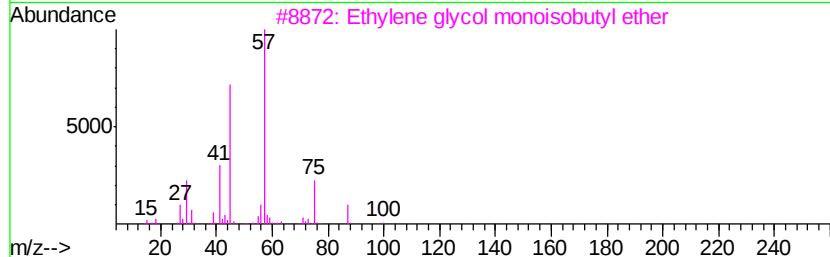
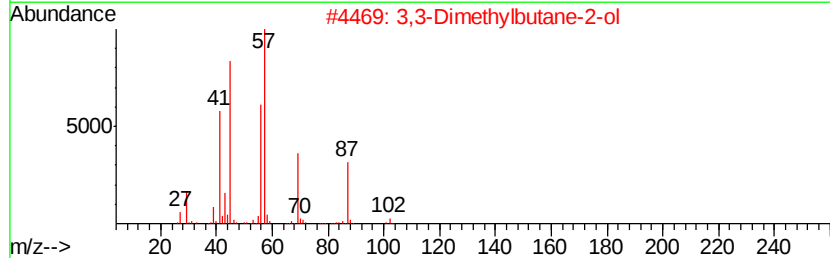
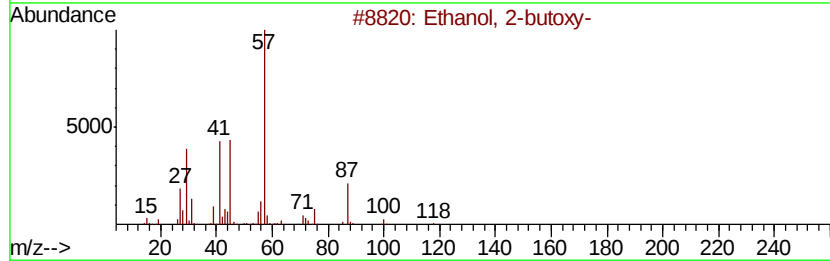
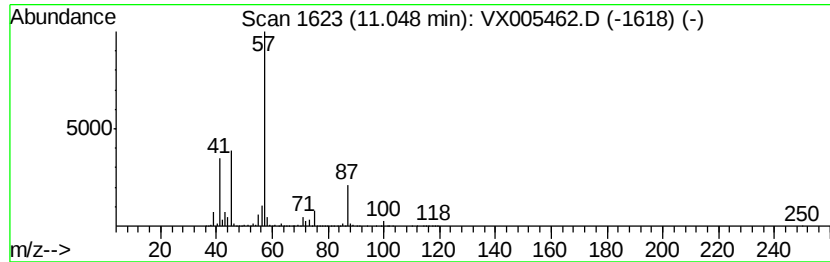
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Ethanol, 2-butoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.05	93.19 ug/l	1784770	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-butoxy-	118	C6H14O2	000111-76-2	91
2		3,3-Dimethylbutane-2-ol	102	C6H14O	000464-07-3	64
3		Ethylene glycol monoisobutyl ether	118	C6H14O2	004439-24-1	53
4		Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
5		Propanoic acid, 2-hydroxyethyl e...	118	C5H10O3	024567-27-9	40



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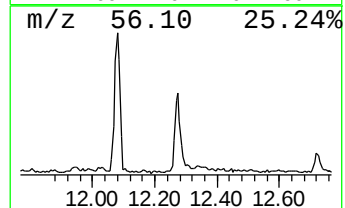
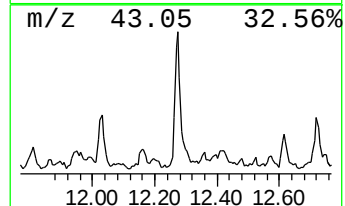
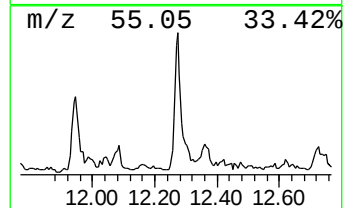
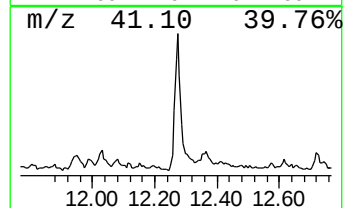
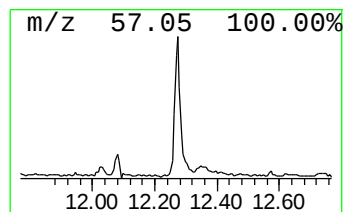
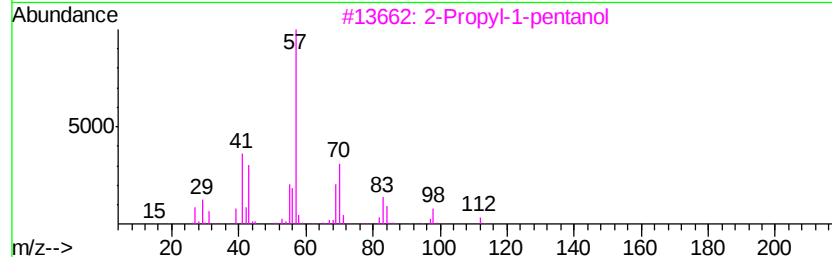
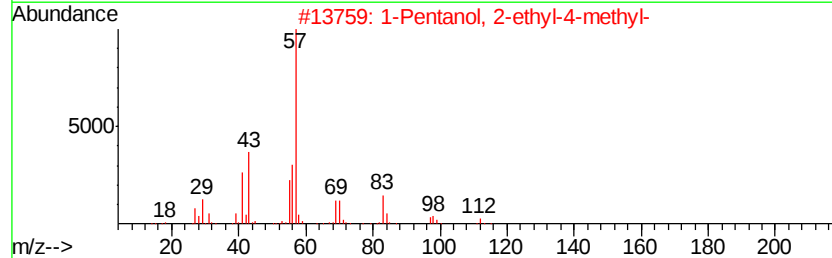
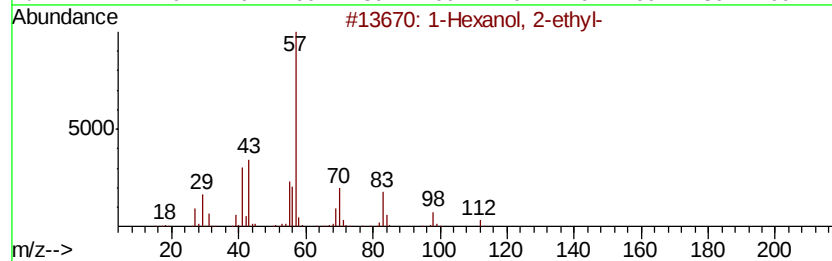
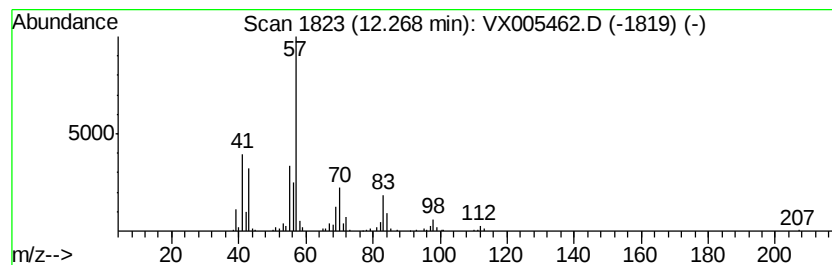
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Peak Number 4 1-Hexanol, 2-ethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.27	5.46 ug/l	104046	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	90
2	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	50
3	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	47
4	3-Undecene, 6-methyl-, (E)-	168	C12H24	074630-52-7	43
5	2-Ethyl-1-hexanol, methyl ether	144	C9H20O	1000365-10-2	42



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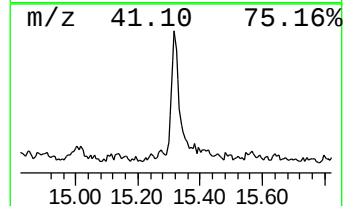
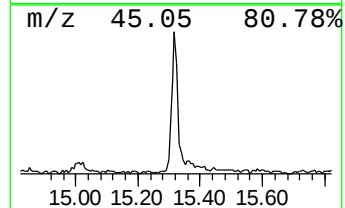
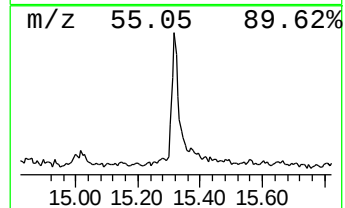
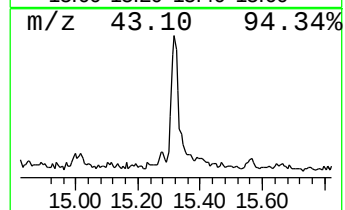
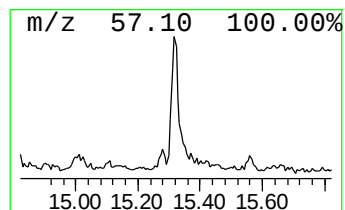
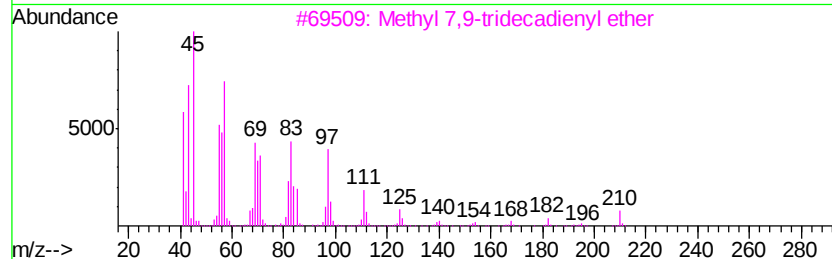
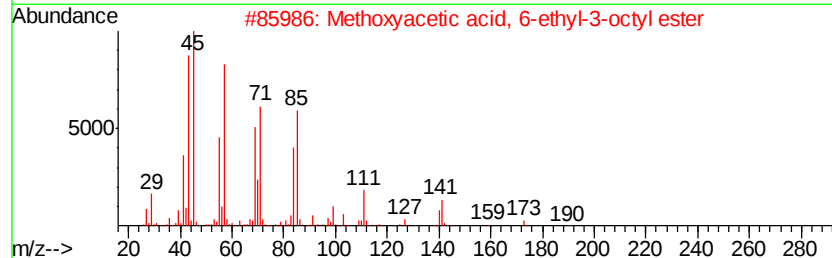
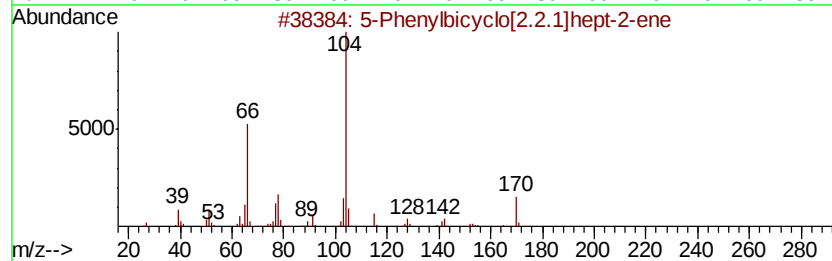
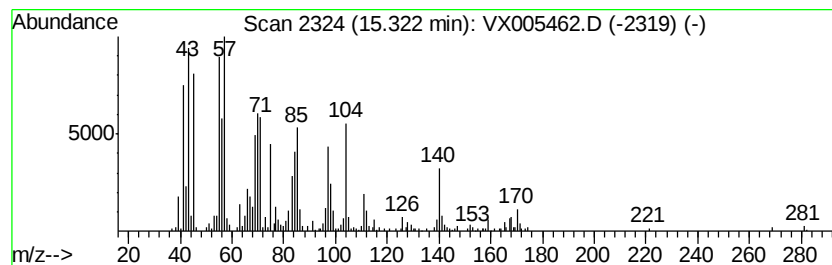
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Peak Number 5 5-Phenylbicyclo[2.2.1]hept-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.32	6.57 ug/l	125180	1,4-Dichlorobenzene-d4	12.08	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	5-Phenylbicyclo[2.2.1]hept-2-ene	170	C13H14	006143-30-2	78
2	Methoxyacetic acid, 6-ethyl-3-oc...	230	C13H26O3	1000282-69-8	25
3	Methyl 7,9-tridecadienyl ether	210	C14H26O	1000131-00-0	22
4	1-Dodecene	168	C12H24	000112-41-4	15
5	1-Tridecene	182	C13H26	002437-56-1	11



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX101918\
Data File : VX005462.D
Acq On : 19 Oct 2018 17:00
Operator : JC/MD
Sample : J5604-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MS-VB-29736-BOX-2

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X101218W.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
Isopropyl Alcohol	2.62	13.7	ug/l	187439	1	5.67	686443	50.0
1-Butanol	7.32	21.4	ug/l	357239	2	6.86	835019	50.0
Ethanol, 2-butoxy-	11.05	93.2	ug/l	1784770	3	10.12	957622	50.0
1-Hexanol, 2-ethyl-	12.27	5.5	ug/l	104046	4	12.08	953295	50.0
5-Phenylbicyclo[2...	15.32	6.6	ug/l	125180	4	12.08	953295	50.0