

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX052820\
 Data File : VX016474.D
 Acq On : 28 May 2020 10:59
 Operator : JC/SP
 Sample : L2738-03 10X
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 25-28-COMP

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\82X052720W.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	1.471	59	63	73	rVB	173651	197184	8.45%	0.933%
2	2.081	157	163	179	rBV	674287	1023024	43.86%	4.841%
3	2.325	198	203	212	rBV	61917	103098	4.42%	0.488%
4	2.416	212	218	225	rBV	45857	74850	3.21%	0.354%
5	3.910	453	463	478	rBV	529851	1339022	57.41%	6.337%
6	4.294	516	526	539	rBV2	20564	57768	2.48%	0.273%
7	4.635	573	582	596	rBV2	29604	97429	4.18%	0.461%
8	5.464	703	718	732	rBV	188800	545873	23.40%	2.583%
9	5.629	732	745	761	rVB	345505	975134	41.81%	4.615%
10	6.031	798	811	825	rBV	213764	562275	24.11%	2.661%
11	6.830	930	942	959	rBV	546558	1283358	55.02%	6.073%
12	7.635	1066	1074	1080	rBV2	30131	62550	2.68%	0.296%
13	8.696	1241	1248	1255	rBV	1197549	1793063	76.88%	8.485%
14	9.561	1385	1390	1396	rBV	36092	48813	2.09%	0.231%
15	10.098	1472	1478	1495	rVB	1157549	1595215	68.39%	7.549%
16	10.896	1605	1609	1614	rVB	21634	27761	1.19%	0.131%
17	11.122	1640	1646	1657	rBV	1029063	1283989	55.05%	6.076%
18	11.512	1706	1710	1720	rVB	64087	88925	3.81%	0.421%
19	11.610	1720	1726	1730	rBV	65848	83785	3.59%	0.397%
20	11.793	1752	1756	1764	rVB	21983	30680	1.32%	0.145%
21	11.872	1764	1769	1773	rBV	26325	39103	1.68%	0.185%
22	11.963	1780	1784	1789	rVB	132565	160383	6.88%	0.759%
23	12.061	1795	1800	1807	rVB	1357201	1633695	70.04%	7.731%
24	12.140	1808	1813	1823	rVB	464532	595612	25.54%	2.819%
25	12.256	1827	1832	1844	rBV	360215	546800	23.44%	2.588%
26	12.353	1844	1848	1857	rVB6	22812	49349	2.12%	0.234%
27	12.457	1863	1865	1870	rVB	26028	28815	1.24%	0.136%
28	12.506	1870	1873	1879	rVB	25365	35446	1.52%	0.168%
29	12.890	1932	1936	1944	rVB	307761	361436	15.50%	1.710%
30	13.012	1951	1956	1965	rBV	190801	304010	13.03%	1.439%
31	13.109	1968	1972	1974	rVV	213912	281489	12.07%	1.332%
32	13.140	1974	1977	1994	rVB	484200	786731	33.73%	3.723%
33	13.304	2000	2004	2007	rVB	53021	55872	2.40%	0.264%
34	13.457	2025	2029	2040	rBV	1670180	2332415	100.00%	11.038%

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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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Title : SW846 8260

35	13.548	2040	2044	2053	rVB	128419	213472	9.15%	1.010%
36	13.725	2069	2073	2075	rBV	162369	201519	8.64%	0.954%
37	13.792	2081	2084	2085	rBV	59597	72566	3.11%	0.343%
38	13.810	2085	2087	2096	rVB2	220133	248836	10.67%	1.178%
39	13.902	2097	2102	2104	rBV	99858	147241	6.31%	0.697%
40	13.932	2104	2107	2117	rVB	177940	285034	12.22%	1.349%
41	14.237	2152	2157	2172	rBV	214630	413546	17.73%	1.957%
42	14.365	2175	2178	2182	rVB3	16555	23531	1.01%	0.111%
43	14.444	2187	2191	2194	rBV	97201	109085	4.68%	0.516%
44	14.493	2194	2199	2202	rBV3	51595	64471	2.76%	0.305%
45	14.560	2207	2210	2214	rVB	82478	89757	3.85%	0.425%
46	14.676	2224	2229	2234	rVB	79707	110134	4.72%	0.521%
47	14.822	2250	2253	2257	rVB	37551	51239	2.20%	0.242%
48	15.469	2355	2359	2364	rVB4	20876	33832	1.45%	0.160%
49	15.609	2377	2382	2388	rBV	370284	546371	23.43%	2.586%
50	15.792	2409	2412	2417	rVB6	21174	35458	1.52%	0.168%

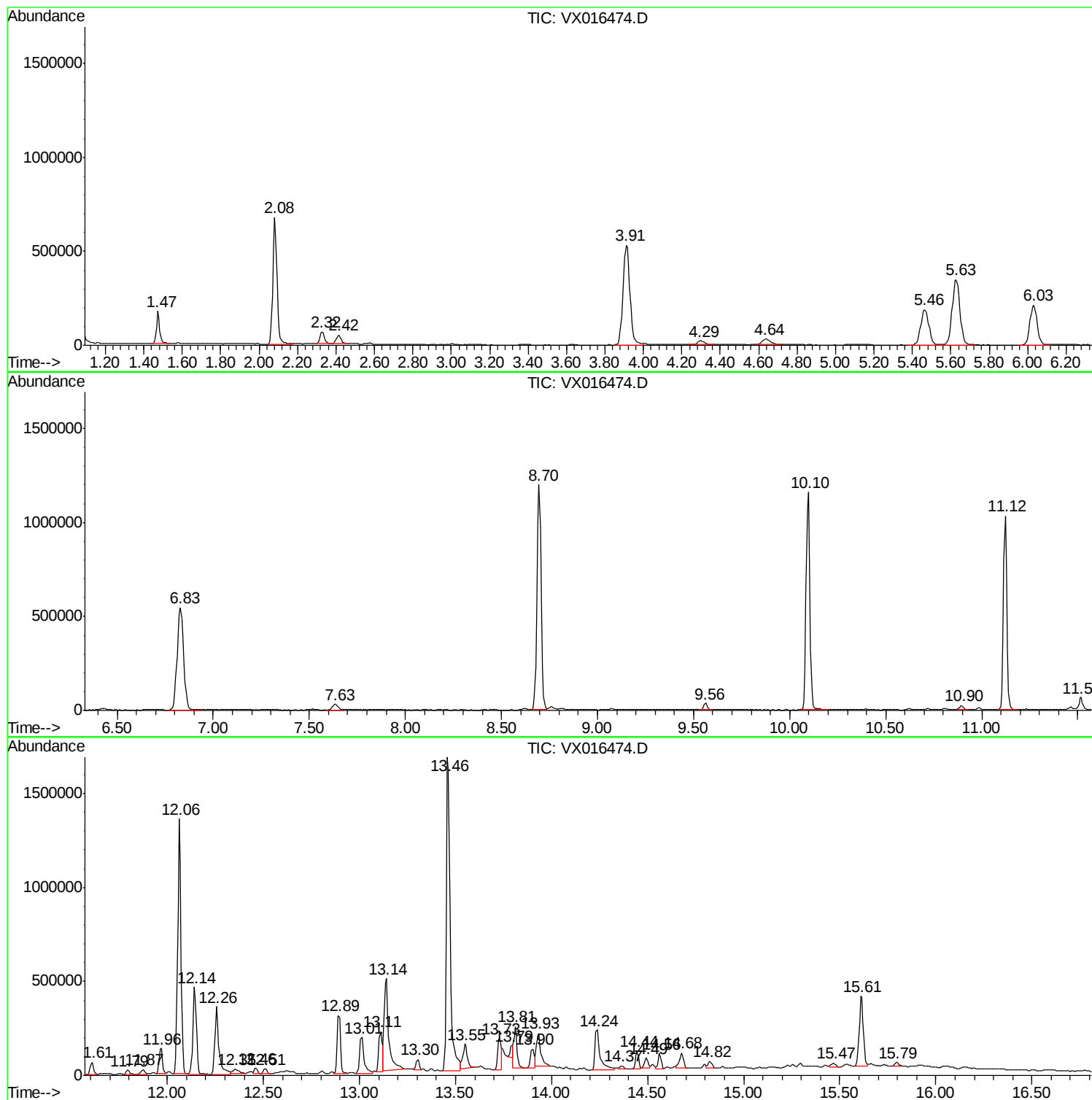
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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



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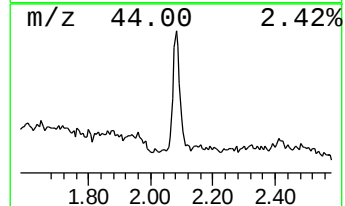
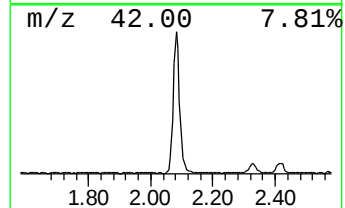
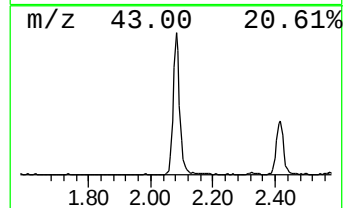
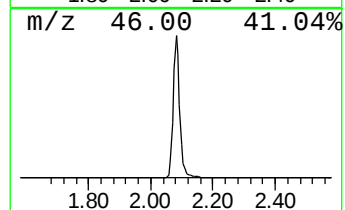
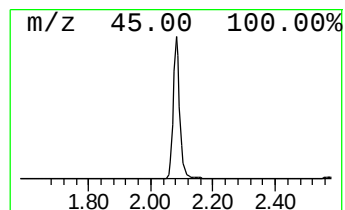
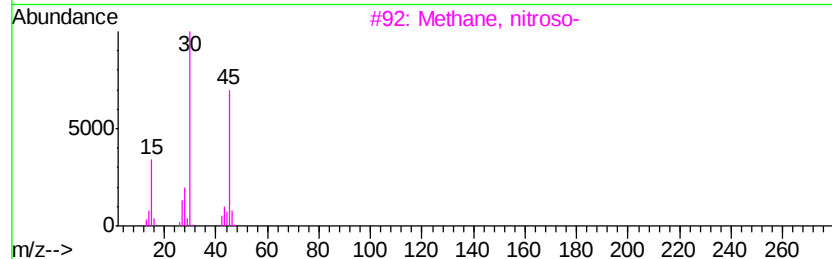
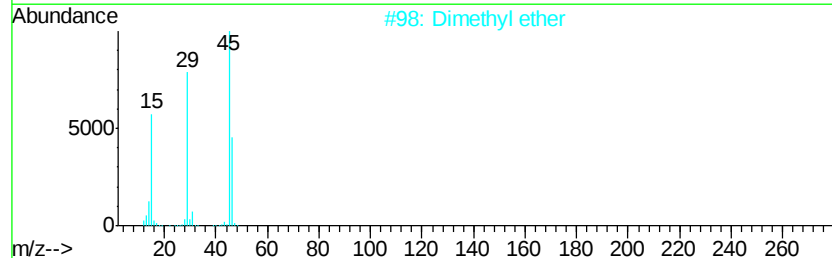
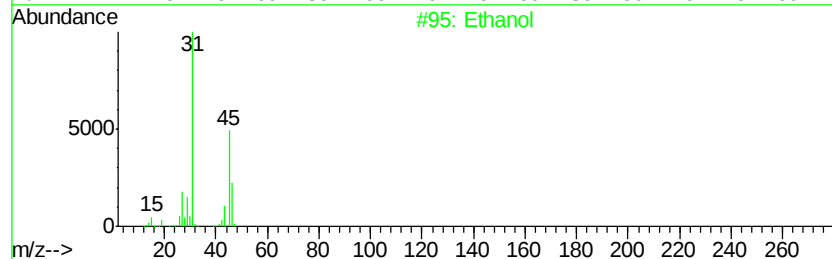
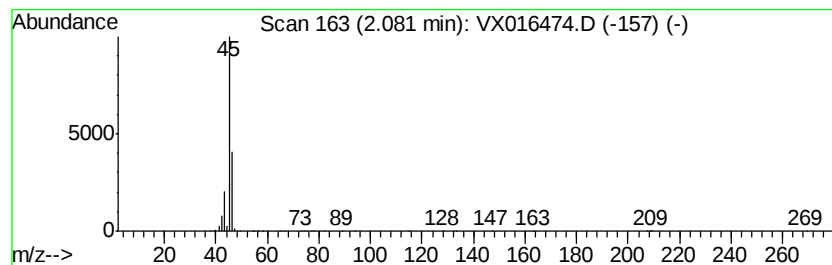
Instrument :
MSVOA_X
ClientSampled :
25-28-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.		
2.08	52.46 ug/l	1023020	Pentafluorobenzene	5.62		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol		46	C2H6O	000064-17-5	78
2	Dimethyl ether		46	C2H6O	000115-10-6	9
3	Methane, nitroso-		45	CH3NO	000865-40-7	4
4	Formic acid		46	CH2O2	000064-18-6	4
5	Oxalic acid		90	C2H2O4	000144-62-7	4



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Instrument :
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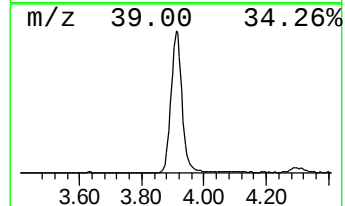
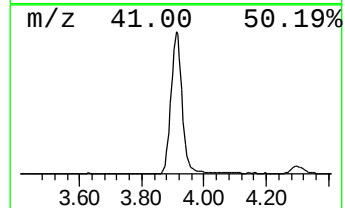
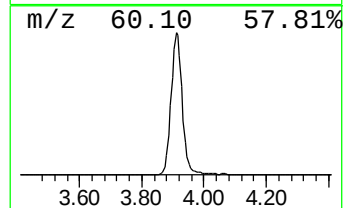
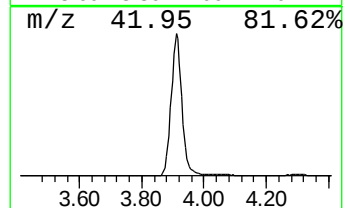
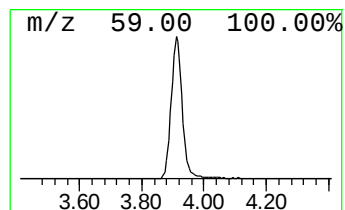
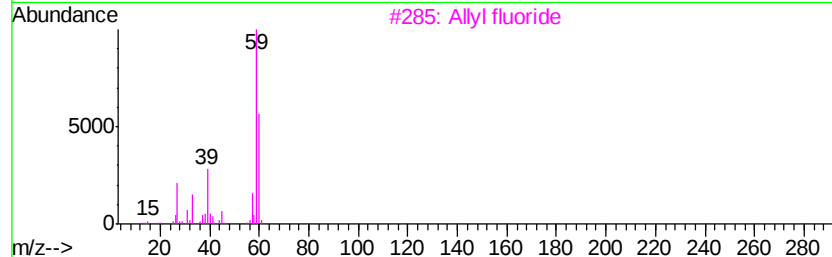
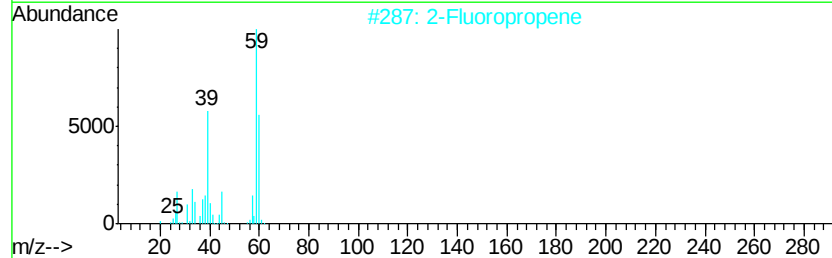
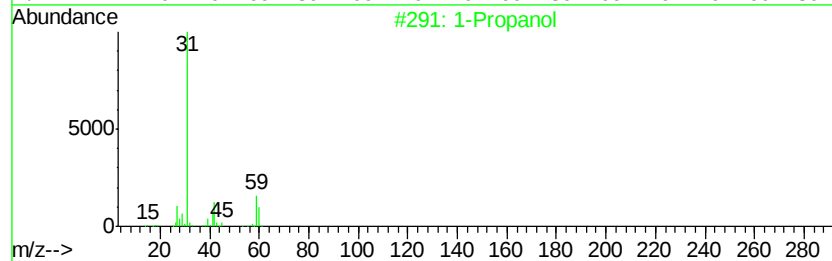
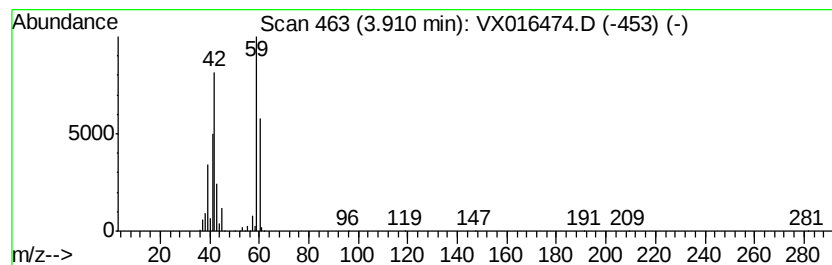
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.91	68.66 ug/l	1339020	Pentafluorobenzene	5.62

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Propanol	60	C3H8O	000071-23-8	78
2		2-Fluoropropene	60	C3H5F	001184-60-7	47
3		Allyl fluoride	60	C3H5F	000818-92-8	38
4		Cyclopropane	42	C3H6	000075-19-4	9
5		Methanamine, N-hydroxy-N-methyl-	61	C2H7NO	005725-96-2	9



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Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 4 Sample Multiplier: 1

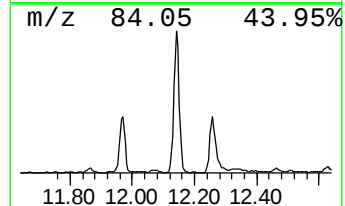
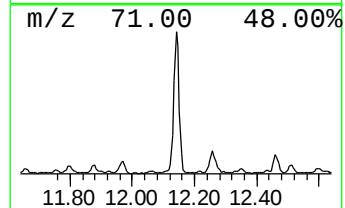
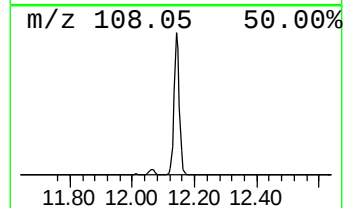
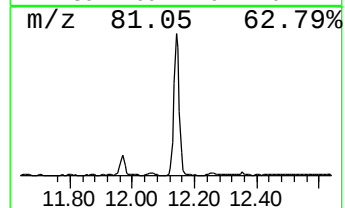
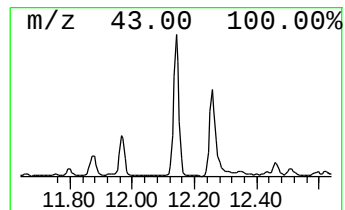
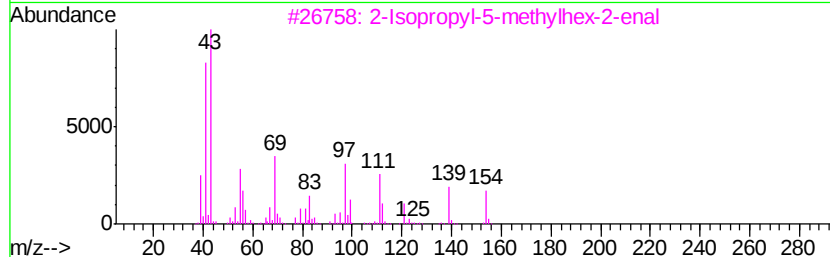
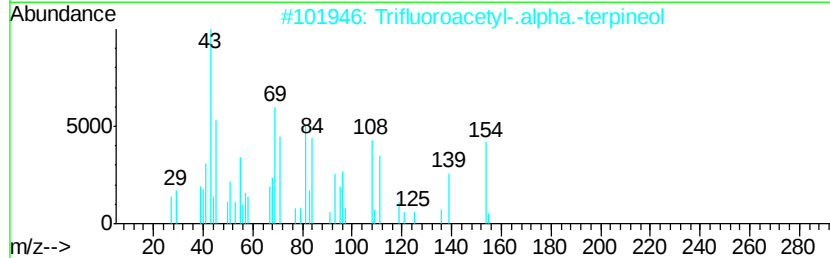
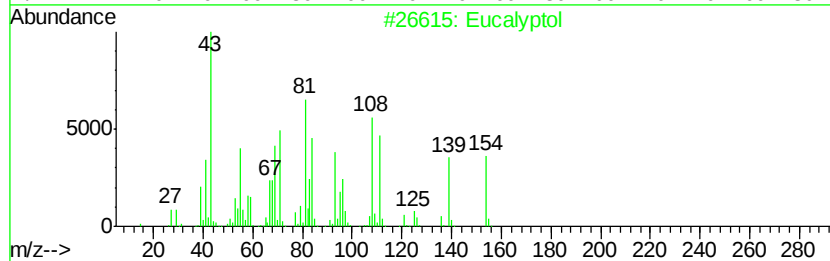
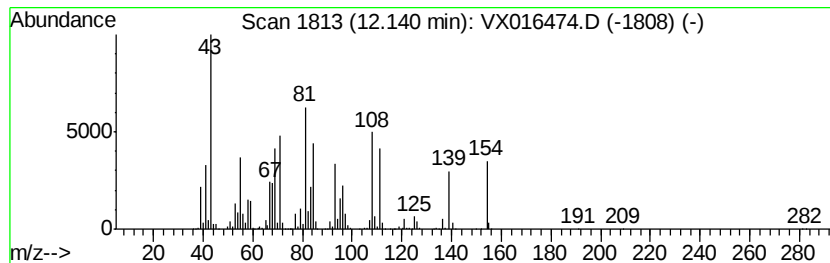
Instrument :
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ClientSampled :
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 4 Eucalyptol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.14	18.23 ug/l	595612	1,4-Dichlorobenzene-d4	12.06	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eucalyptol	154	C10H18O	000470-82-6	99
2	Trifluoroacetyl-.alpha.-terpineol	250	C12H17F3O2	1000058-17-6	58
3	2-Isopropyl-5-methylhex-2-enal	154	C10H18O	035158-25-9	27
4	2-Acetylcyclopentanone	126	C7H10O2	001670-46-8	25
5	3-Hepten-2-one, 3-propyl-	154	C10H18O	032064-69-0	25



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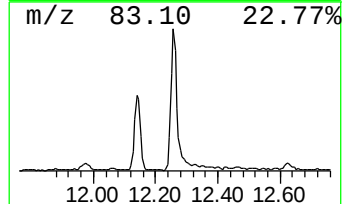
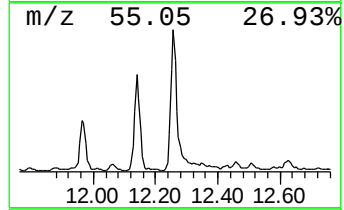
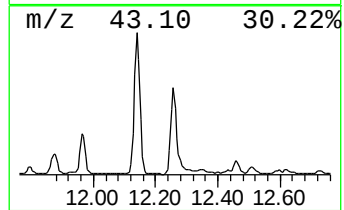
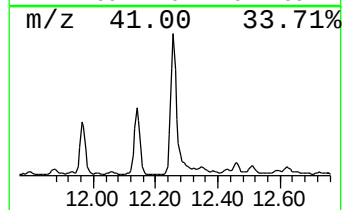
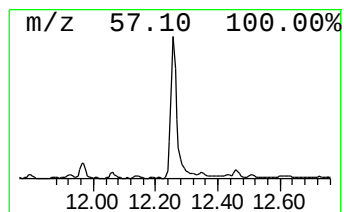
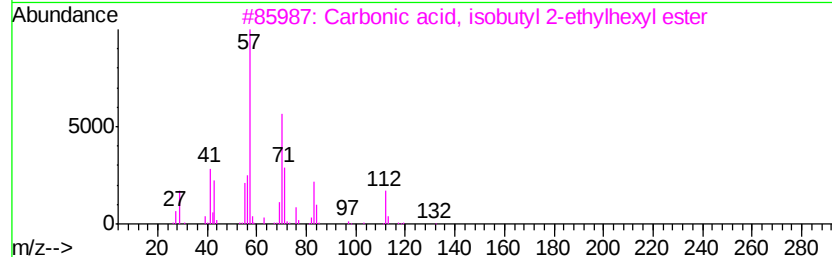
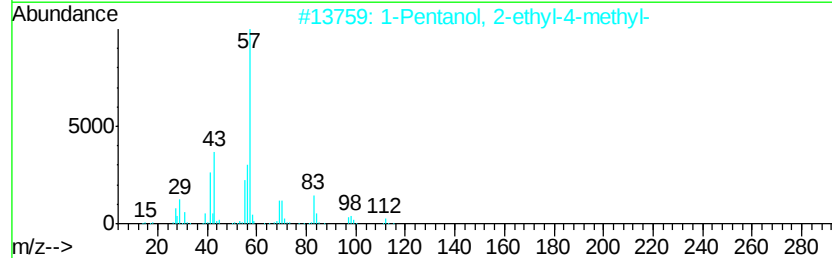
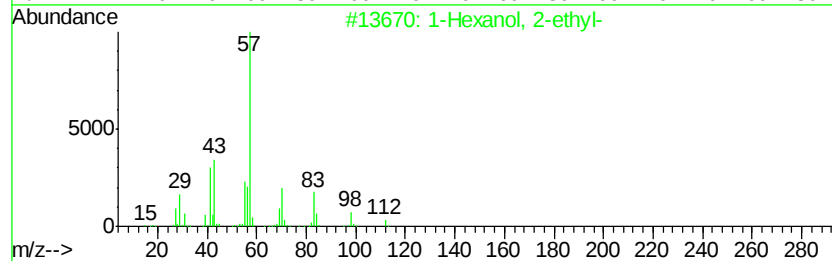
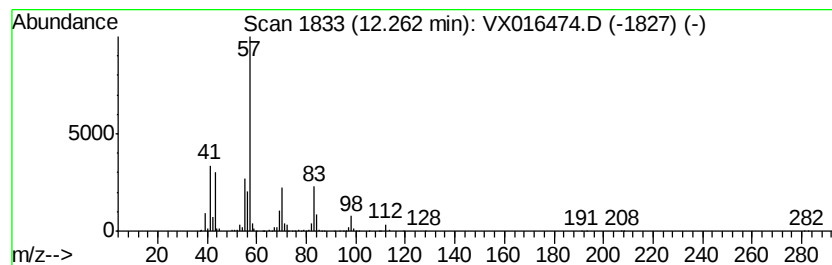
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	16.74 ug/l	546800	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
2		1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	59
3		Carbonic acid, isobutyl 2-ethylhexyl...	230	C13H26O3	1000357-82-9	59
4		Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	53
5		2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50



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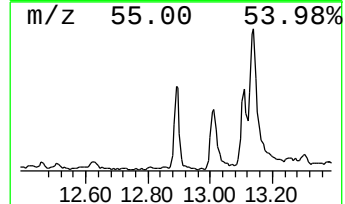
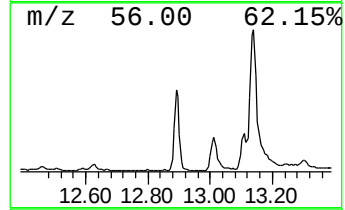
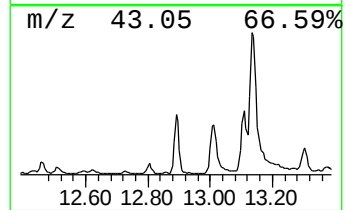
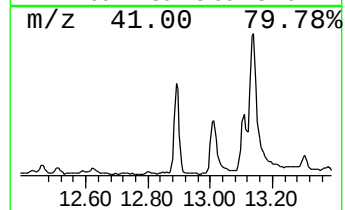
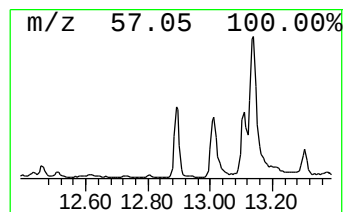
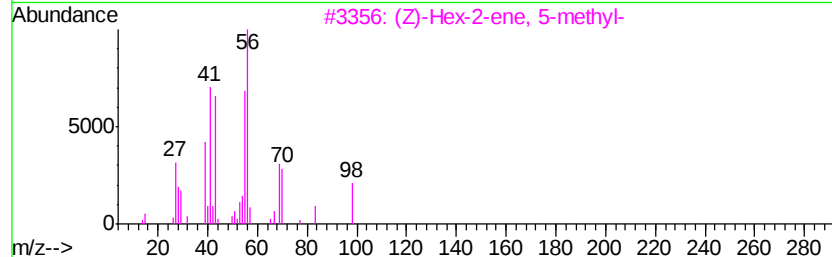
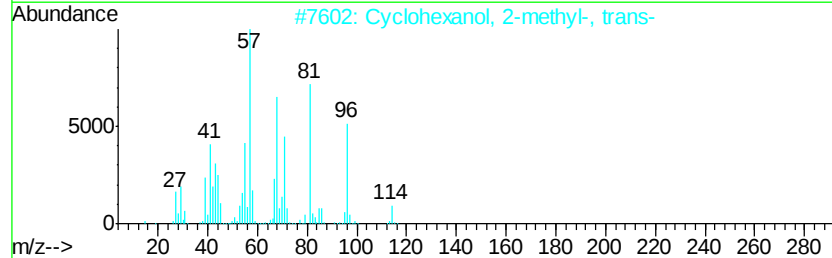
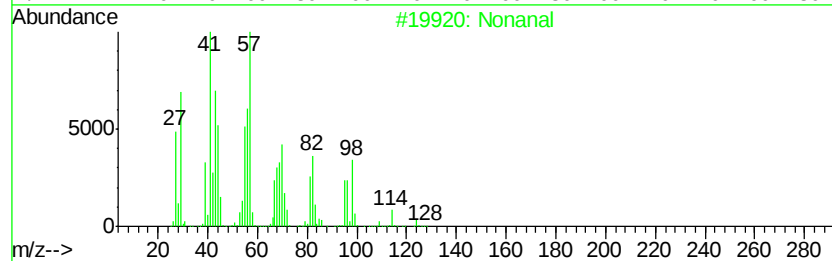
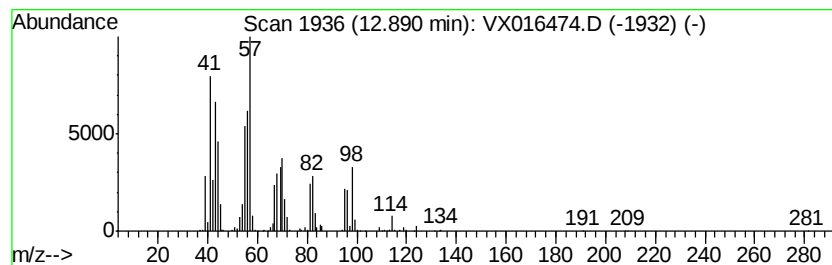
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Quant Title : SW846 8260

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

Peak Number 6 Nonanal Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.89	11.06 ug/l	361436	1,4-Dichlorobenzene-d4	12.06

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal		142	C9H18O	000124-19-6	91
2	Cyclohexanol, 2-methyl-, trans-		114	C7H14O	007443-52-9	46
3	(Z)-Hex-2-ene, 5-methyl-		98	C7H14	013151-17-2	22
4	Heptane, 2-chloro-		134	C7H15Cl	001001-89-4	22
5	5-Methyl-2-hexene,c&t		98	C7H14	003404-62-4	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX052820\
Data File : VX016474.D
Acq On : 28 May 2020 10:59
Operator : JC/SP
Sample : L2738-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
25-28-COMP

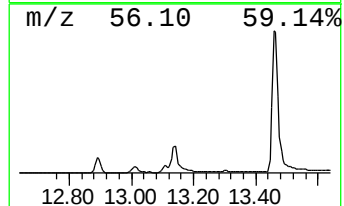
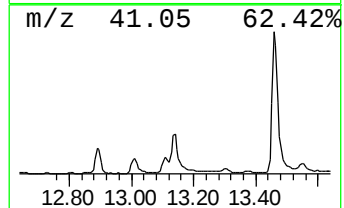
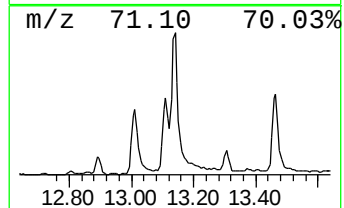
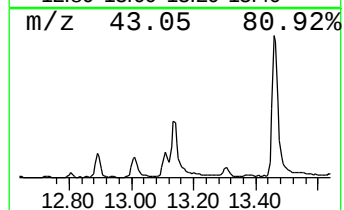
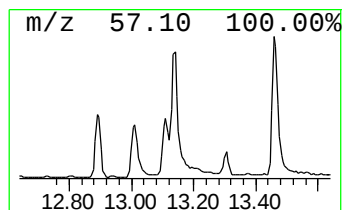
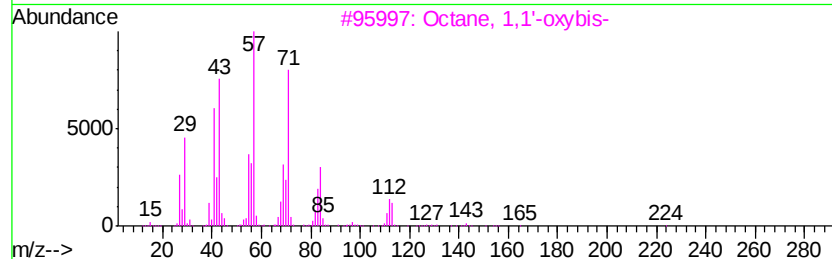
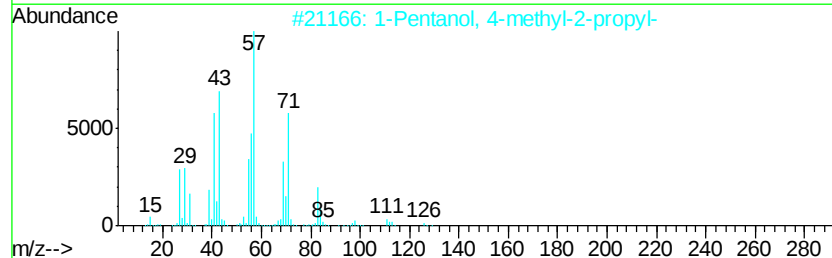
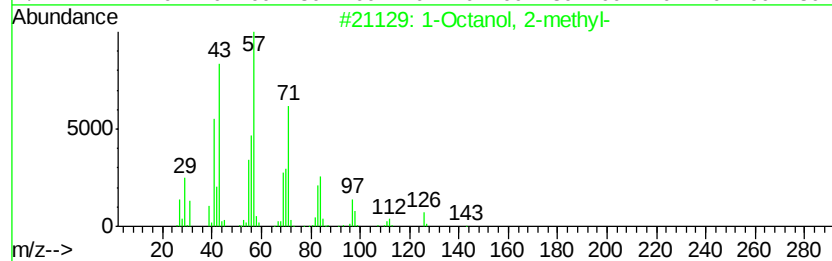
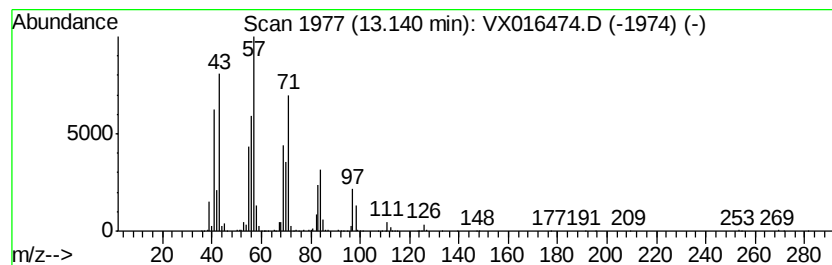
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Quant Title : SW846 8260

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

Peak Number 7 1-Octanol, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.14	24.08 ug/l	786731	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Octanol, 2-methyl-	144	C9H20O	000818-81-5	78
2		1-Pentanol, 4-methyl-2-propyl-	144	C9H20O	054004-41-0	59
3		Octane, 1,1'-oxybis-	242	C16H34O	000629-82-3	59
4		Decane, 1-fluoro-	160	C10H21F	000334-56-5	53
5		1-Fluorononane	146	C9H19F	000463-18-3	53



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX052820\
Data File : VX016474.D
Acq On : 28 May 2020 10:59
Operator : JC/SP
Sample : L2738-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 4 Sample Multiplier: 1

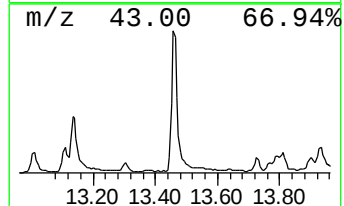
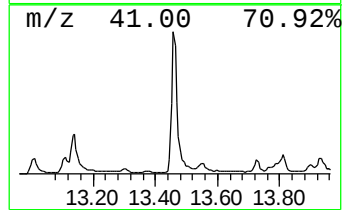
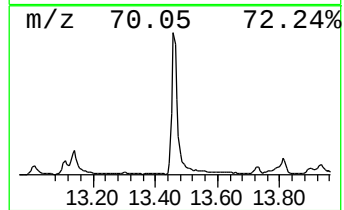
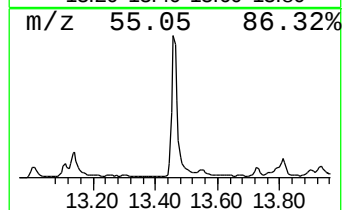
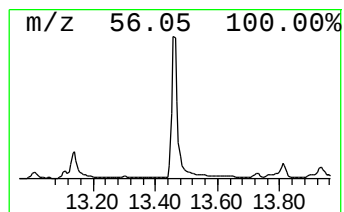
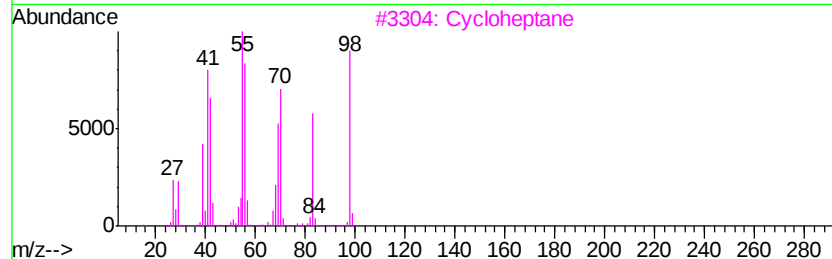
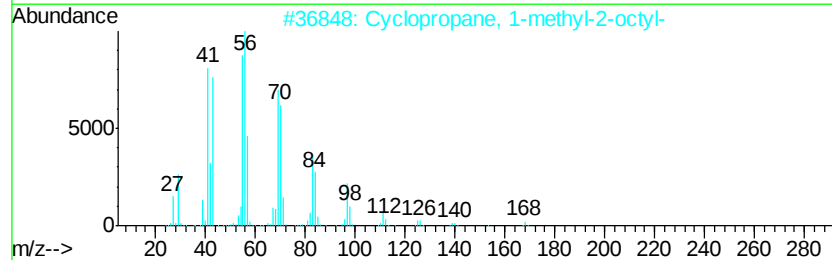
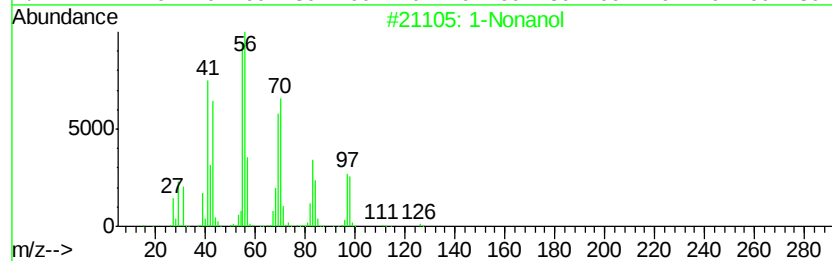
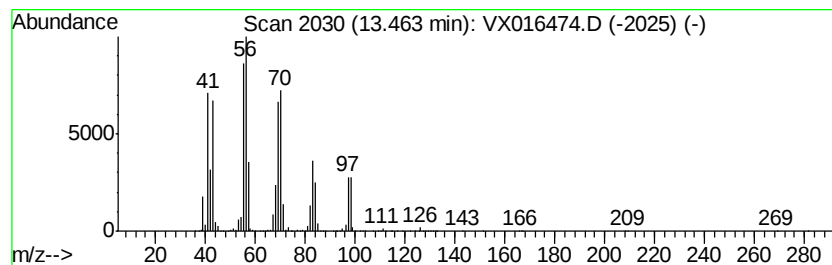
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ClientSampled :
25-28-COMP

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.M
Quant Title : SW846 8260

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

Peak Number 8 1-Nonanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.46	71.38 ug/l	2332420	1,4-Dichlorobenzene-d4	12.06
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	1-Nonanol		144 C9H20O	000143-08-8 91
2	Cyclopropane, 1-methyl-2-octyl-		168 C12H24	037617-26-8 80
3	Cycloheptane		98 C7H14	000291-64-5 74
4	Cyclopropane, 1-methyl-2-pentyl-		126 C9H18	041977-37-1 74
5	Isopropylcyclobutane		98 C7H14	000872-56-0 68



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX052820\
Data File : VX016474.D
Acq On : 28 May 2020 10:59
Operator : JC/SP
Sample : L2738-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
25-28-COMP

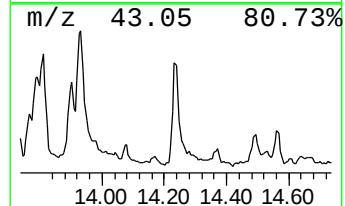
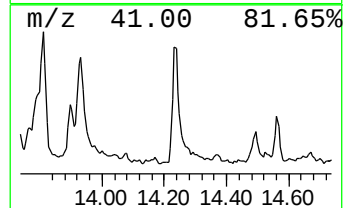
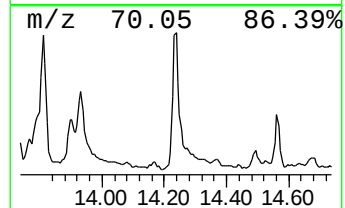
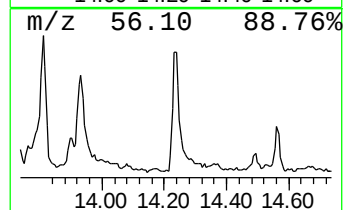
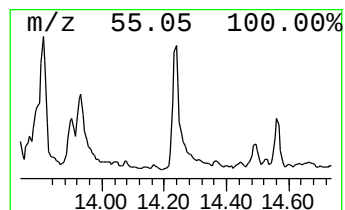
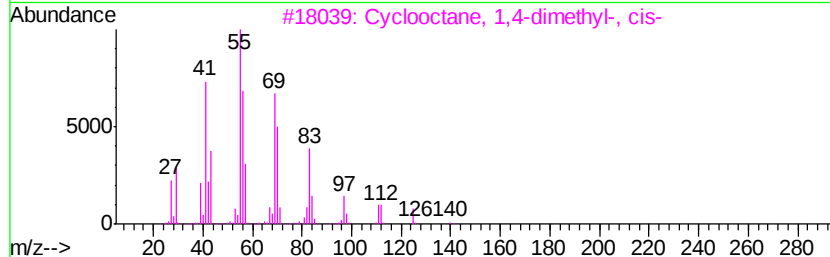
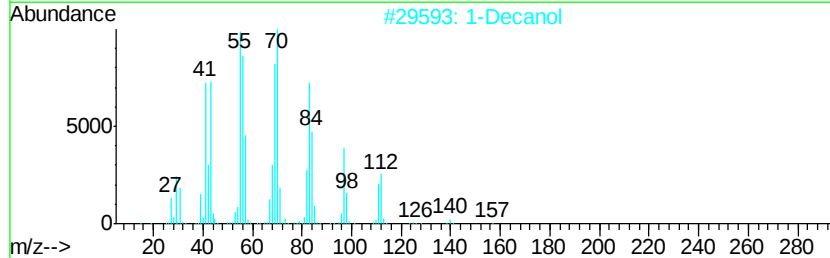
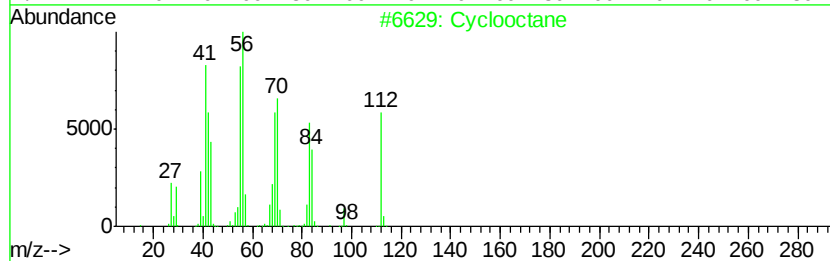
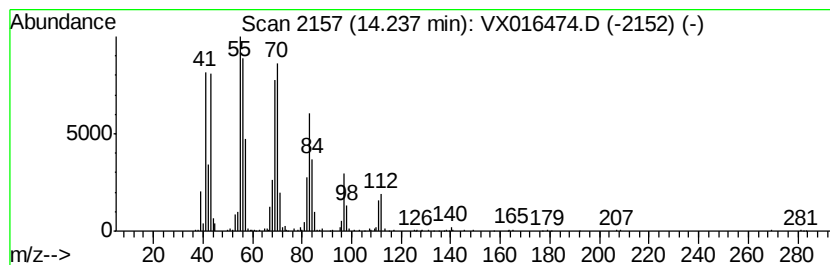
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Quant Title : SW846 8260

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

Peak Number 9 Cyclooctane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.24	12.66 ug/l	413546	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclooctane	112	C8H16	000292-64-8	91
2		1-Decanol	158	C10H22O	000112-30-1	91
3		Cyclooctane, 1,4-dimethyl-, cis-	140	C10H20	013151-99-0	91
4		Carbonochloridic acid, decyl ester	220	C11H21ClO2	055488-51-2	90
5		2-Dodecene, (Z)-	168	C12H24	007206-26-0	90



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX052820\
Data File : VX016474.D
Acq On : 28 May 2020 10:59
Operator : JC/SP
Sample : L2738-03 10X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
25-28-COMP

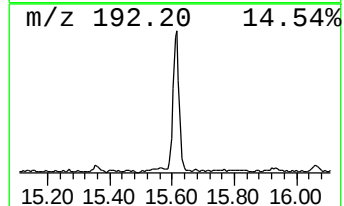
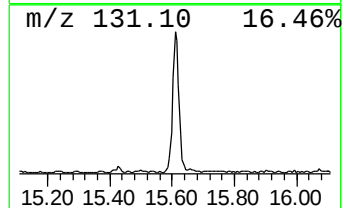
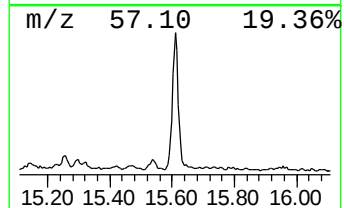
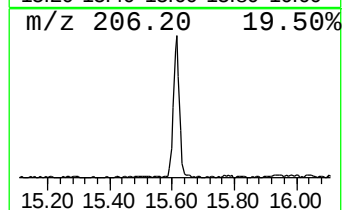
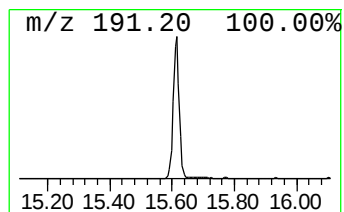
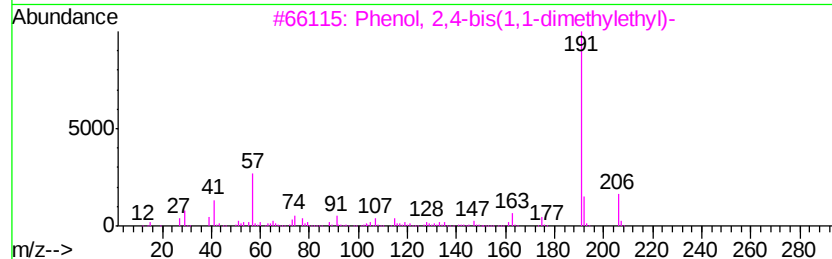
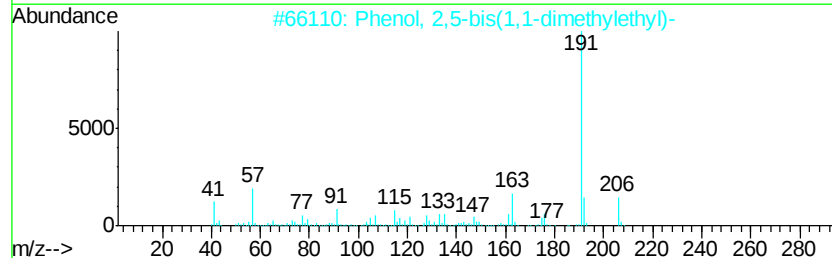
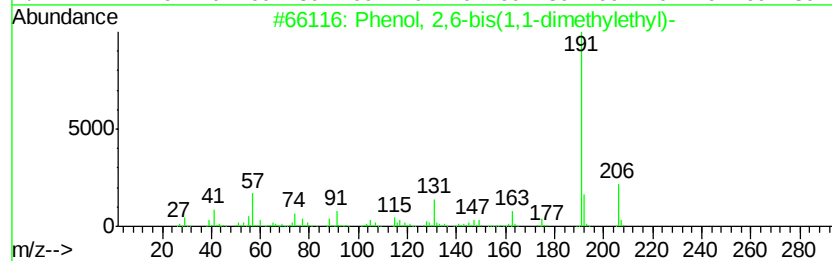
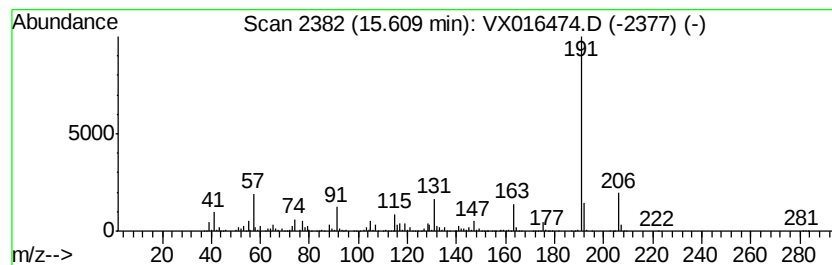
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Quant Title : SW846 8260

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

Peak Number 10 Phenol, 2,6-bis(1,1-dimethy... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.61	16.72 ug/l	546371	1,4-Dichlorobenzene-d4	12.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Phenol, 2,6-bis(1,1-dimethylethyl)-	206	C14H22O	000128-39-2	96
2		Phenol, 2,5-bis(1,1-dimethylethyl)-	206	C14H22O	005875-45-6	90
3		Phenol, 2,4-bis(1,1-dimethylethyl)-	206	C14H22O	000096-76-4	87
4		Ethyl 4-t-butylbenzoate	206	C13H18O2	005406-57-5	81
5		2H-Indeno[1,2-b]furan-2-one, 3,3...	206	C13H18O2	1000196-74-3	80



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX052820\
Data File : VX016474.D
Acq On : 28 May 2020 10:59
Operator : JC/SP
Sample : L2738-03 10X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
25-28-COMP

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X052720W.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
Ethanol	2.08	52.5	ug/l	1023020	1	5.62	975134	50.0
1-Propanol	3.91	68.7	ug/l	1339020	1	5.62	975134	50.0
Eucalyptol	12.14	18.2	ug/l	595612	4	12.06	1633700	50.0
1-Hexanol, 2-ethyl-	12.26	16.7	ug/l	546800	4	12.06	1633700	50.0
Nonanal	12.89	11.1	ug/l	361436	4	12.06	1633700	50.0
1-Octanol, 2-methyl-	13.14	24.1	ug/l	786731	4	12.06	1633700	50.0
1-Nonanol	13.46	71.4	ug/l	2332420	4	12.06	1633700	50.0
Cyclooctane	14.24	12.7	ug/l	413546	4	12.06	1633700	50.0
Phenol, 2,6-bis(1...	15.61	16.7	ug/l	546371	4	12.06	1633700	50.0