

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091620\
 Data File : VX018442.D
 Acq On : 16 Sep 2020 16:05
 Operator : JC/SP
 Sample : L3988-25
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FC-MW1011-20200910

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\82X082120W.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	5.464	706	718	732	rBV2	278475	826219	15.92%	3.508%
2	5.635	735	746	757	rBV	472930	1326447	25.55%	5.632%
3	6.031	801	811	826	rBV2	304621	809850	15.60%	3.439%
4	6.324	847	859	871	rBV	227517	679611	13.09%	2.886%
5	6.830	932	942	955	rBV	708530	1696500	32.68%	7.204%
6	7.659	1072	1078	1086	rVB2	28952	61005	1.18%	0.259%
7	8.037	1128	1140	1149	rBV	264091	515804	9.94%	2.190%
8	8.159	1152	1160	1170	rVV	457949	884441	17.04%	3.756%
9	8.470	1205	1211	1219	rBV	149778	254134	4.90%	1.079%
10	8.696	1236	1248	1255	rBV	1491788	2336229	45.01%	9.920%
11	9.025	1296	1302	1308	rVB	43709	69997	1.35%	0.297%
12	9.604	1392	1397	1404	rBV	260641	508304	9.79%	2.158%
13	9.659	1404	1406	1415	rVB	50341	93256	1.80%	0.396%
14	10.098	1473	1478	1488	rVB2	1549027	2462440	47.44%	10.456%
15	10.323	1510	1515	1523	rVB5	35882	75699	1.46%	0.321%
16	11.000	1622	1626	1630	rBV	57925	73500	1.42%	0.312%
17	11.122	1639	1646	1651	rBV	1318059	1621249	31.23%	6.884%
18	11.756	1742	1750	1753	rBV	54610	71897	1.39%	0.305%
19	11.902	1767	1774	1776	rBV	65662	84595	1.63%	0.359%
20	11.927	1776	1778	1783	rVB	54173	72306	1.39%	0.307%
21	12.006	1786	1791	1796	rBV	727623	943919	18.18%	4.008%
22	12.079	1796	1803	1810	rVB2	2780383	5190775	100.00%	22.041%
23	12.280	1832	1836	1841	rVB2	82597	112600	2.17%	0.478%
24	12.378	1841	1852	1858	rBV	636097	891997	17.18%	3.788%
25	12.689	1899	1903	1908	rVV3	37489	63217	1.22%	0.268%
26	12.750	1908	1913	1919	rVV4	53338	95388	1.84%	0.405%
27	12.878	1927	1934	1939	rVB	124442	176947	3.41%	0.751%
28	12.939	1939	1944	1947	rBV	43306	58324	1.12%	0.248%
29	13.176	1972	1983	1986	rBV	72898	111023	2.14%	0.471%
30	13.628	2052	2057	2060	rVV	185850	244496	4.71%	1.038%
31	13.676	2060	2065	2067	rVV4	88971	185495	3.57%	0.788%
32	13.701	2067	2069	2078	rVB	167130	200985	3.87%	0.853%
33	13.792	2079	2084	2087	rBV	59372	75169	1.45%	0.319%
34	13.890	2096	2100	2105	rBV2	39251	57086	1.10%	0.242%

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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	13.963	2105	2112	2116	rBV	151351	227191	4.38%	0.965%
36	14.006	2116	2119	2124	rVB2	77287	107324	2.07%	0.456%
37	14.146	2138	2142	2147	rVB	57536	74068	1.43%	0.315%
38	14.524	2199	2204	2212	rBV4	27105	55473	1.07%	0.236%
39	14.713	2232	2235	2239	rBV4	44150	53179	1.02%	0.226%
40	14.829	2247	2254	2260	rBV	53842	101989	1.96%	0.433%

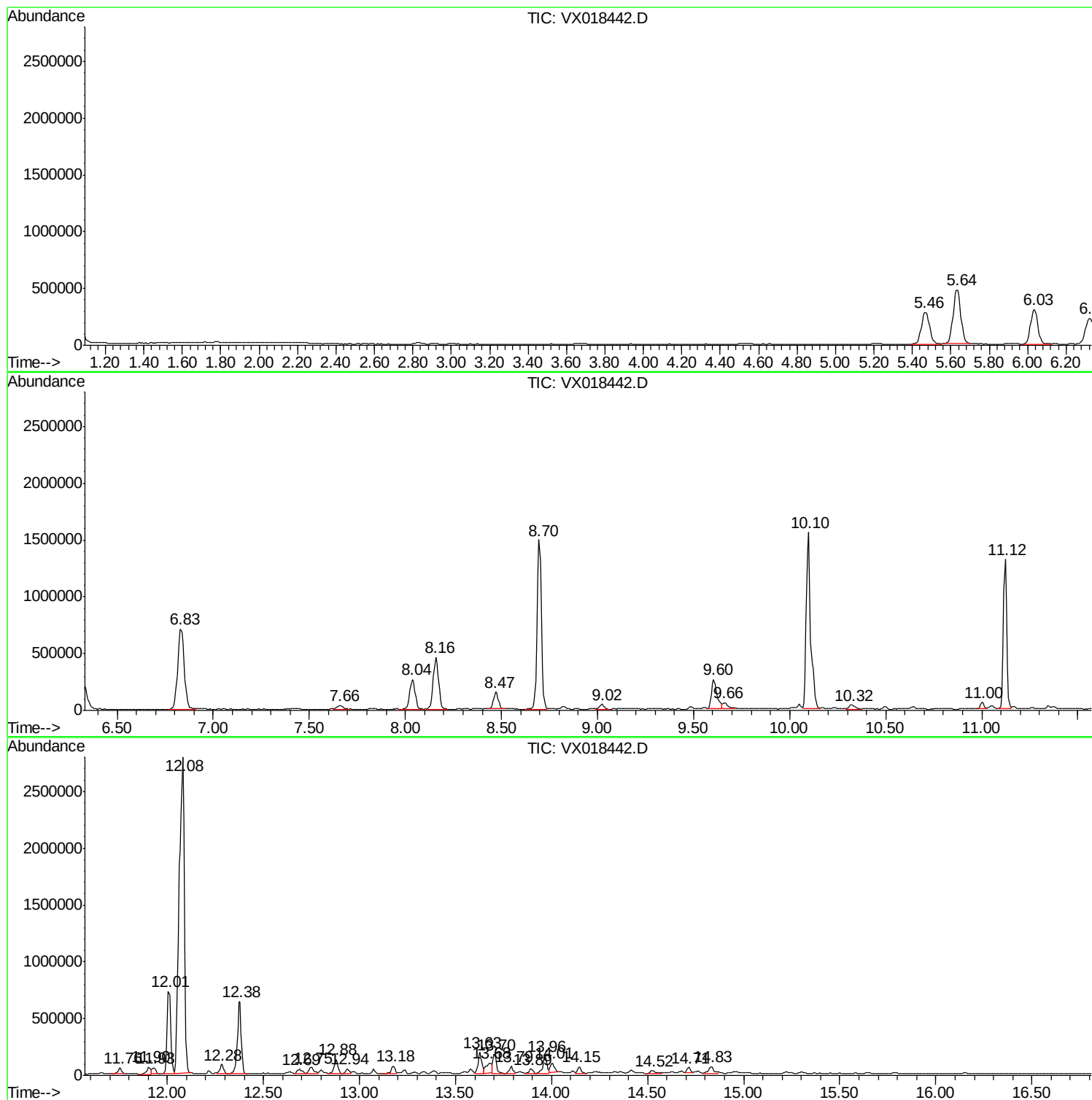
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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



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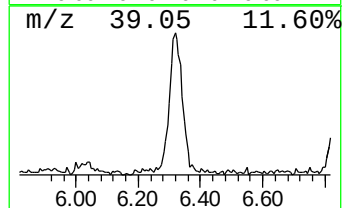
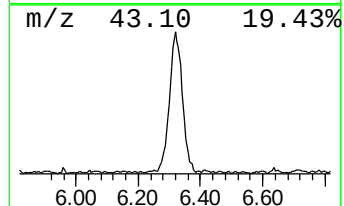
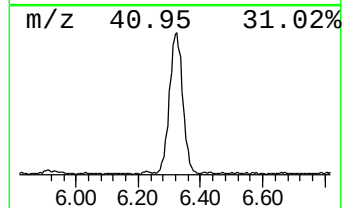
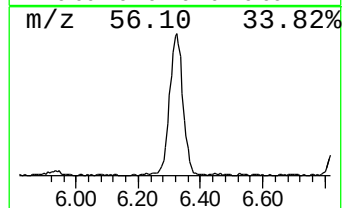
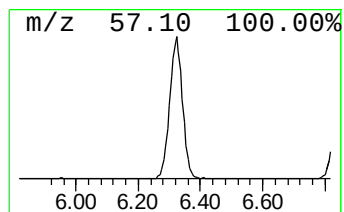
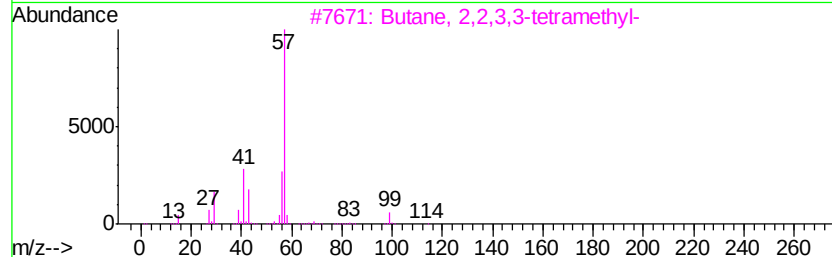
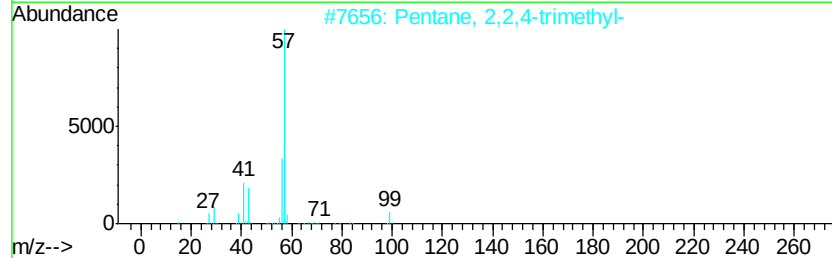
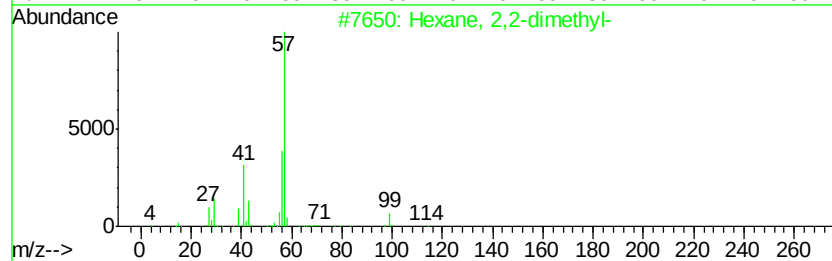
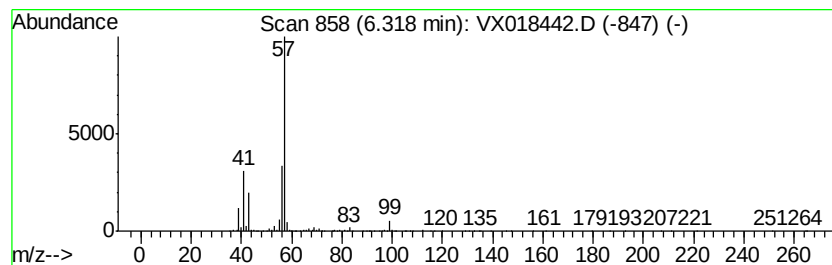
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 1 Hexane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	20.03 ug/l	679611	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	78
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	64
4		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59
5		Hexane, 2,2,5-trimethyl-	128	C9H20	003522-94-9	59



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ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FC-MW10I1-20200910

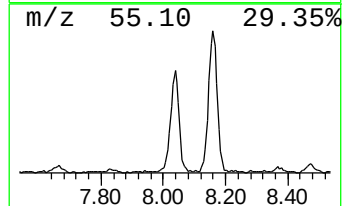
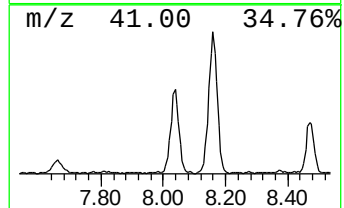
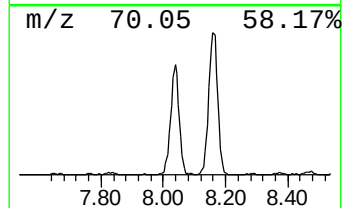
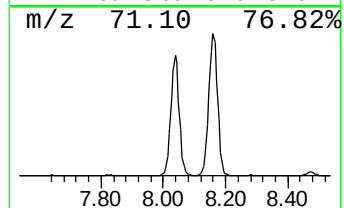
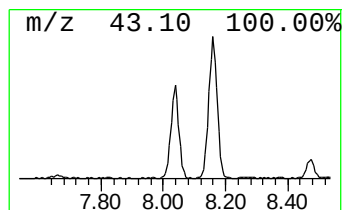
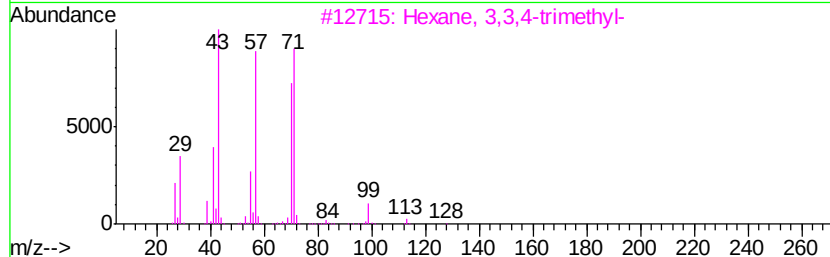
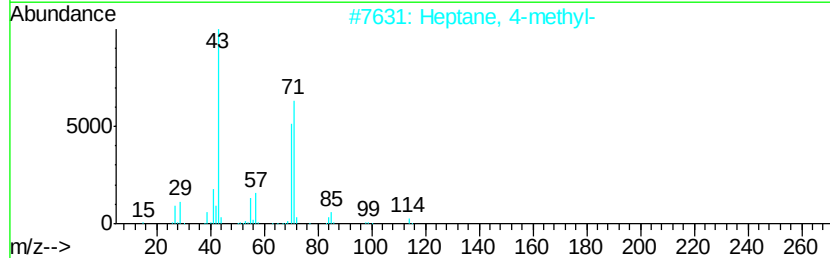
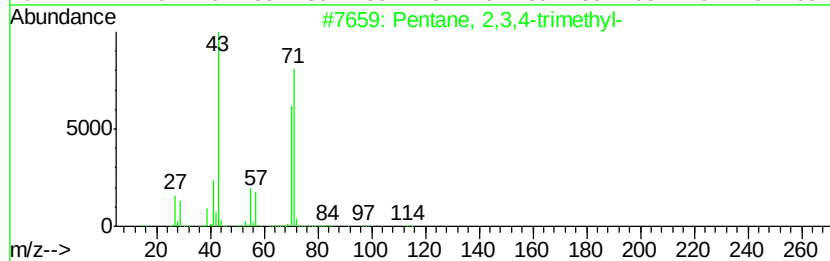
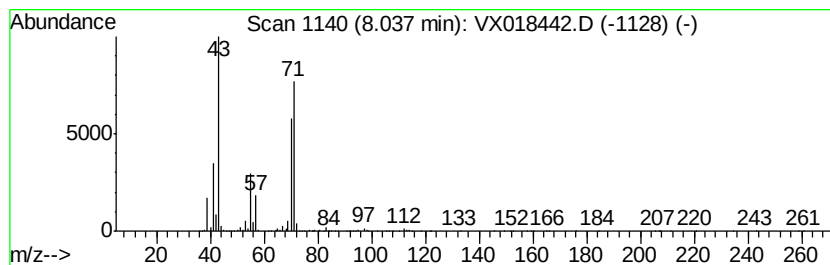
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	15.20 ug/l	515804	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	90
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
4		S-(Neopentylthiocarbonyl)thio...	179	C6H13NOS2	035659-84-8	53
5		Hexane, 3,3,4,4-tetramethyl-	142	C10H22	005171-84-6	50



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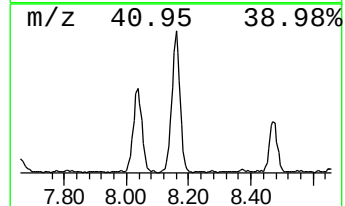
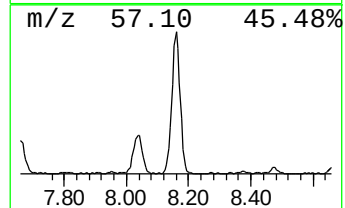
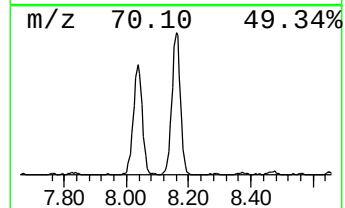
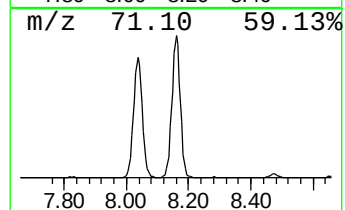
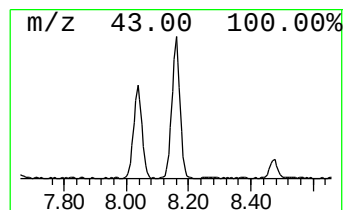
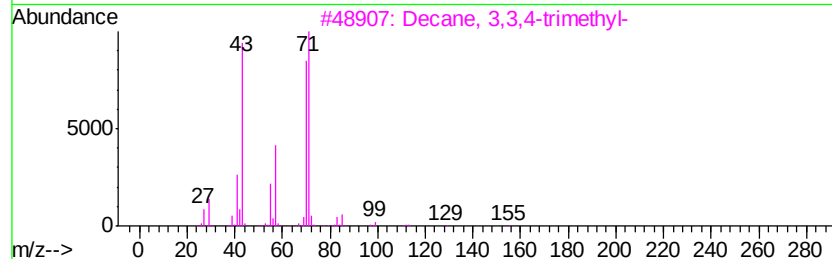
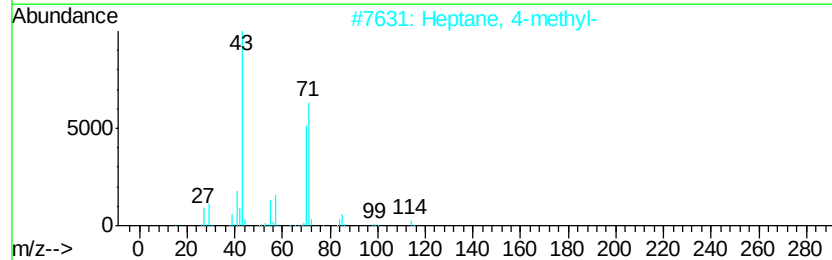
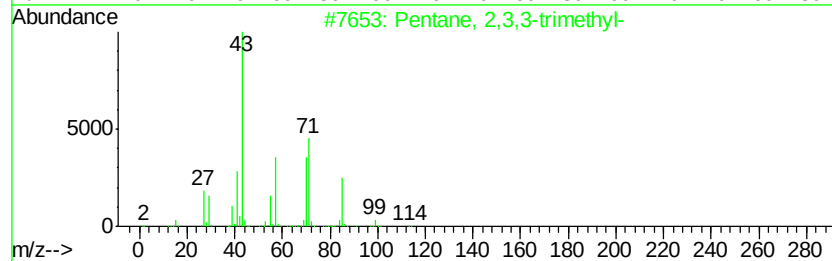
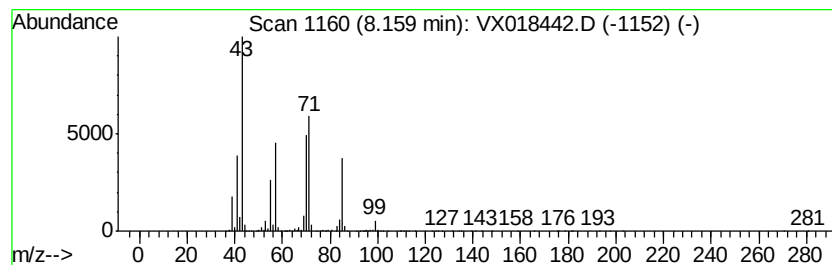
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Quant Title : SW846 8260

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

Peak Number 3 Pentane, 2,3,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.16	26.07 ug/l	884441	1,4-Difluorobenzene	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	59
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	53



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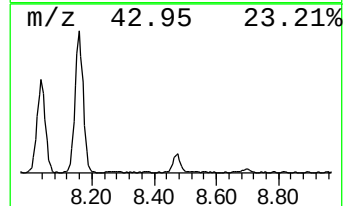
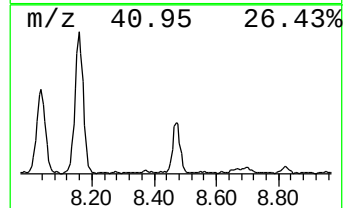
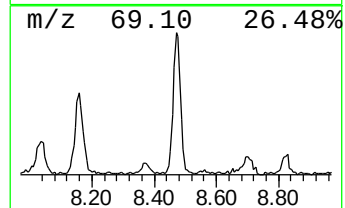
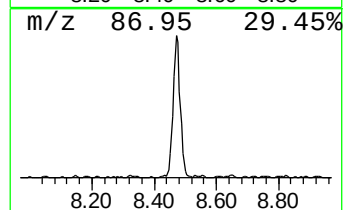
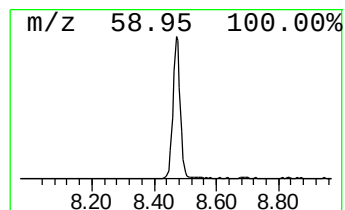
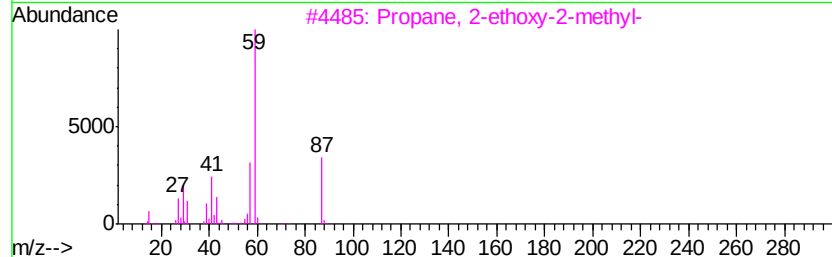
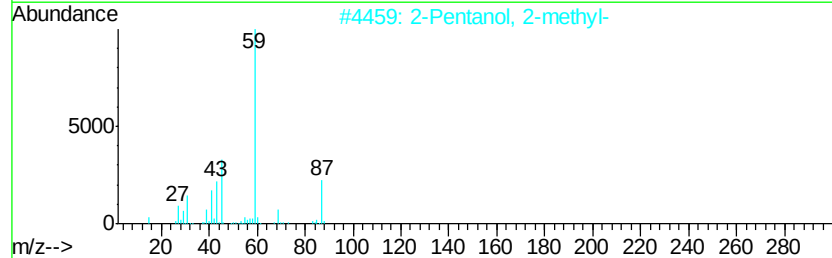
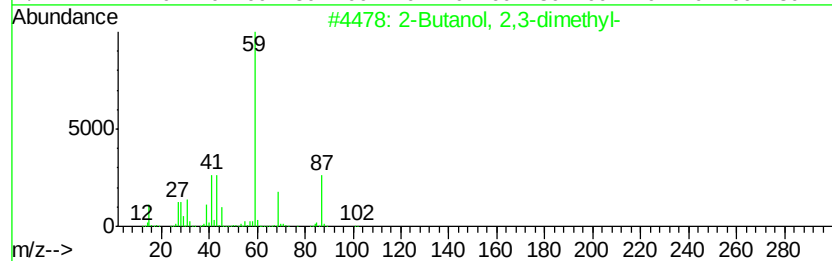
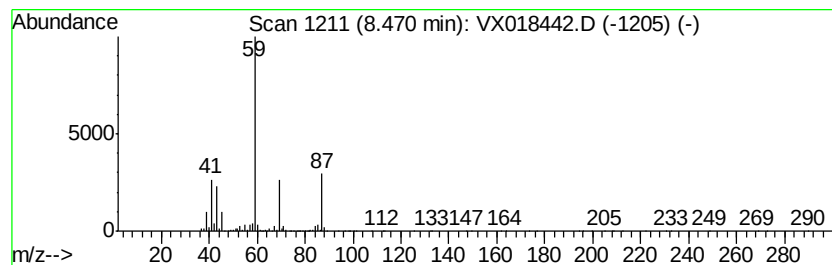
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Quant Title : SW846 8260

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

Peak Number 4 2-Butanol, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	5.16 ug/l	254134	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	72
3		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	64
4		1-(1-Methoxypropan-2-yloxy)propan...	260	C14H28O4	1000367-13-1	42
5		2-Propanol, 1,1'-[(1-methyl-1,2-...	192	C9H20O4	001638-16-0	42



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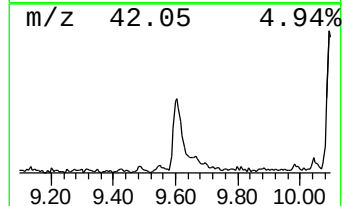
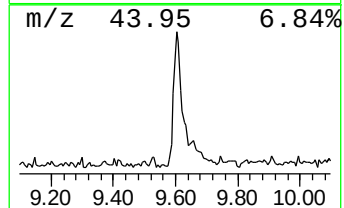
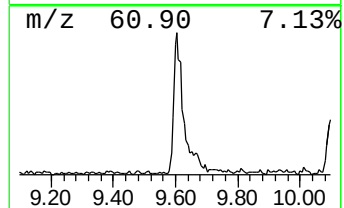
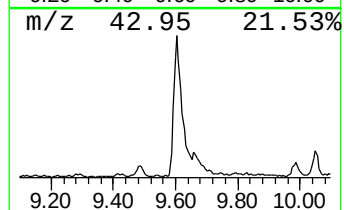
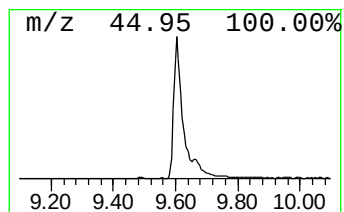
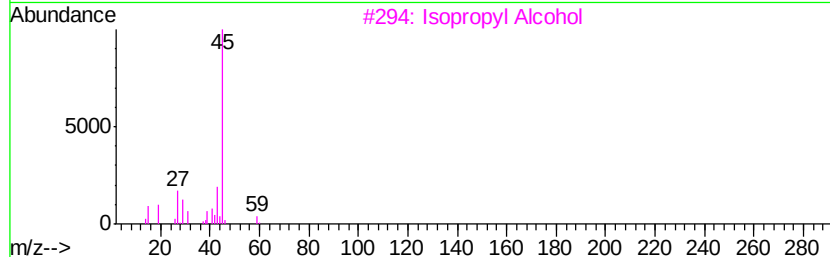
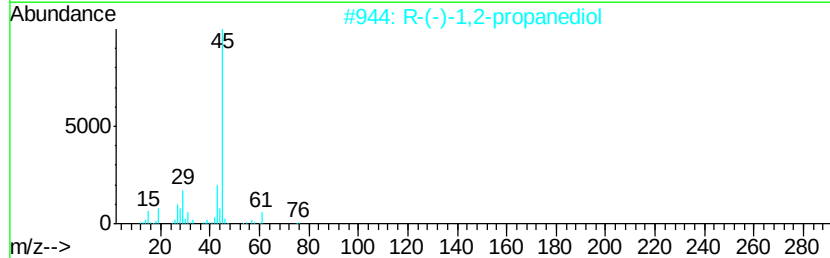
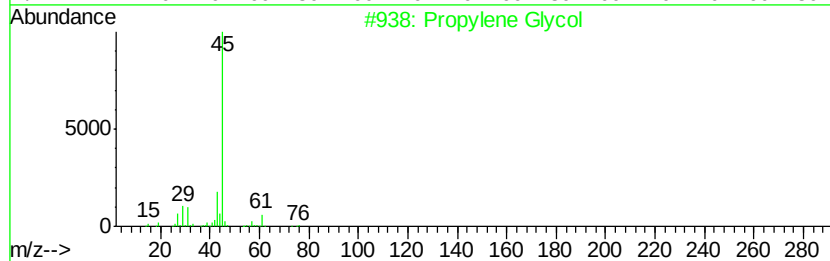
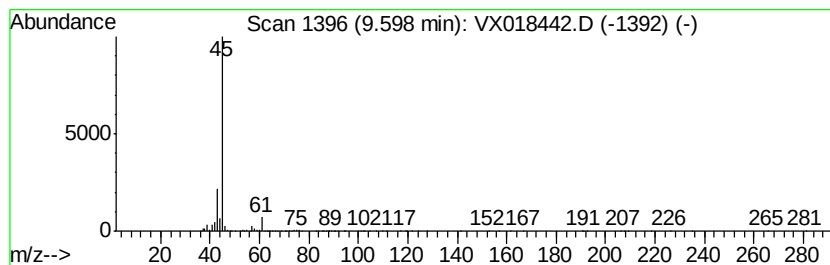
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 5 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	10.32 ug/l	508304	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	86
2		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3		Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5		3-Ethyl-2-pentanol	116	C7H16O	000609-27-8	40



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091620\
Data File : VX018442.D
Acq On : 16 Sep 2020 16:05
Operator : JC/SP
Sample : L3988-25
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FC-MW10I1-20200910

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.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
Hexane, 2,2-dimet...	6.32	20.0	ug/l	679611	2	6.83	1696500	50.0
Pentane, 2,3,4-tr...	8.04	15.2	ug/l	515804	2	6.83	1696500	50.0
Pentane, 2,3,3-tr...	8.16	26.1	ug/l	884441	2	6.83	1696500	50.0
2-Butanol, 2,3-di...	8.47	5.2	ug/l	254134	3	10.10	2462440	50.0
Propylene Glycol	9.60	10.3	ug/l	508304	3	10.10	2462440	50.0