

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX091620\
 Data File : VX018444.D
 Acq On : 16 Sep 2020 16:50
 Operator : JC/SP
 Sample : L3988-27
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FC-DUP06-20200910

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	708	718	732	rBV	278511	800021	15.80%	3.508%
2	5.635	735	746	763	rVB2	468325	1322611	26.12%	5.799%
3	6.031	801	811	822	rBV	303424	790817	15.62%	3.467%
4	6.324	848	859	871	rVB	222394	673071	13.29%	2.951%
5	6.836	931	943	958	rBV	692783	1677710	33.13%	7.356%
6	7.659	1068	1078	1086	rVB2	29215	70323	1.39%	0.308%
7	8.037	1128	1140	1149	rBV	257690	508812	10.05%	2.231%
8	8.159	1153	1160	1171	rVB	446800	872350	17.23%	3.825%
9	8.470	1204	1211	1220	rBV	155118	266117	5.26%	1.167%
10	8.696	1235	1248	1255	rBV	1481143	2319402	45.80%	10.169%
11	9.025	1297	1302	1310	rVB2	43312	72178	1.43%	0.316%
12	9.604	1393	1397	1404	rBV	185224	373784	7.38%	1.639%
13	10.098	1473	1478	1488	rVB2	1521419	2394203	47.28%	10.497%
14	10.317	1509	1514	1525	rVB6	33915	73728	1.46%	0.323%
15	11.000	1622	1626	1630	rBV	56637	73866	1.46%	0.324%
16	11.122	1641	1646	1651	rBV	1304565	1635568	32.30%	7.171%
17	11.756	1742	1750	1755	rBV	51896	77030	1.52%	0.338%
18	11.902	1768	1774	1776	rBV2	63253	87088	1.72%	0.382%
19	11.933	1776	1779	1786	rVB	59890	79313	1.57%	0.348%
20	12.012	1786	1792	1796	rBV	693022	901645	17.81%	3.953%
21	12.079	1796	1803	1811	rVB2	2593788	5063839	100.00%	22.202%
22	12.286	1829	1837	1841	rVB	79316	108939	2.15%	0.478%
23	12.378	1843	1852	1858	rVB	609465	854099	16.87%	3.745%
24	12.683	1899	1902	1908	rVV5	33738	59548	1.18%	0.261%
25	12.750	1908	1913	1918	rVV3	42406	82745	1.63%	0.363%
26	12.878	1927	1934	1939	rVB	124968	175115	3.46%	0.768%
27	12.939	1939	1944	1947	rBV2	39337	55440	1.09%	0.243%
28	13.176	1975	1983	1987	rVV	72395	105310	2.08%	0.462%
29	13.628	2052	2057	2060	rVV2	193061	242659	4.79%	1.064%
30	13.682	2060	2066	2067	rVV3	83320	177312	3.50%	0.777%
31	13.701	2067	2069	2078	rVB	160057	205097	4.05%	0.899%
32	13.792	2079	2084	2087	rBV	58422	72668	1.44%	0.319%
33	13.963	2105	2112	2116	rBV	150889	218618	4.32%	0.959%
34	13.999	2116	2118	2123	rVB2	74983	102803	2.03%	0.451%

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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 >
Peak separation: 5

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35	14.146	2138	2142	2147	rVB	61302	72355	1.43%	0.317%
36	14.713	2231	2235	2239	rBV2	44222	54197	1.07%	0.238%
37	14.829	2248	2254	2258	rBV2	52951	87459	1.73%	0.383%

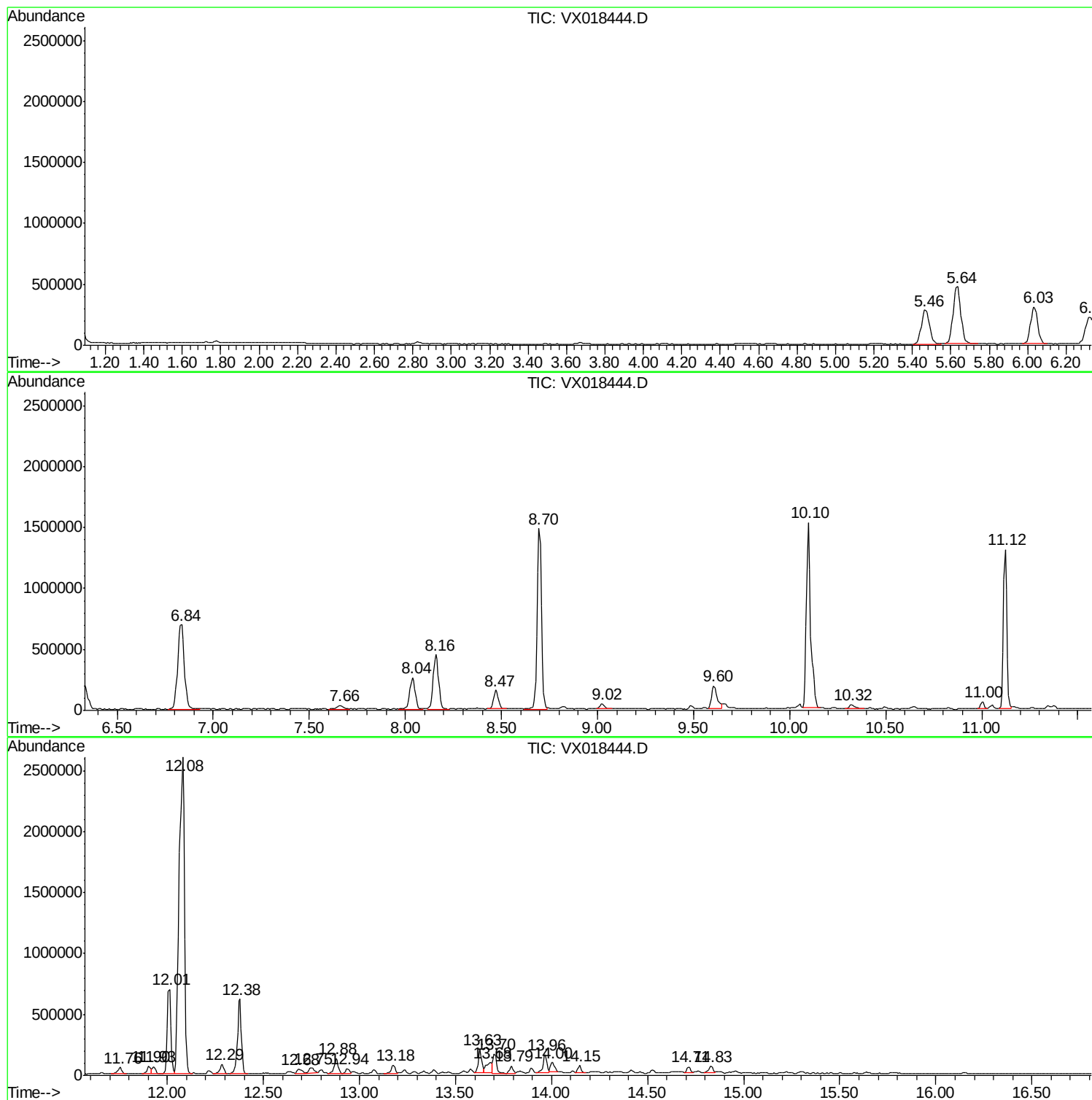
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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



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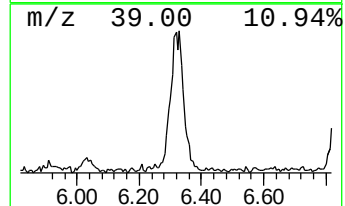
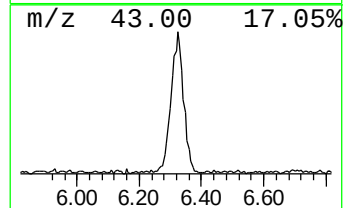
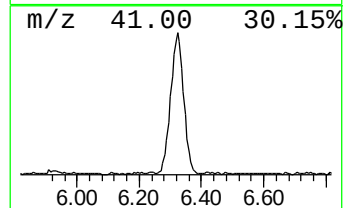
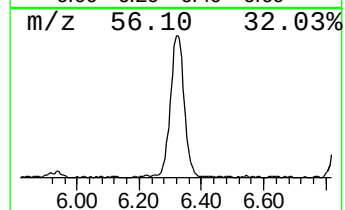
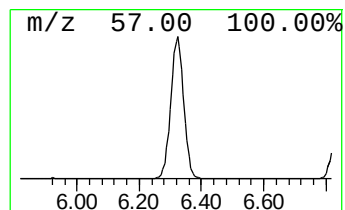
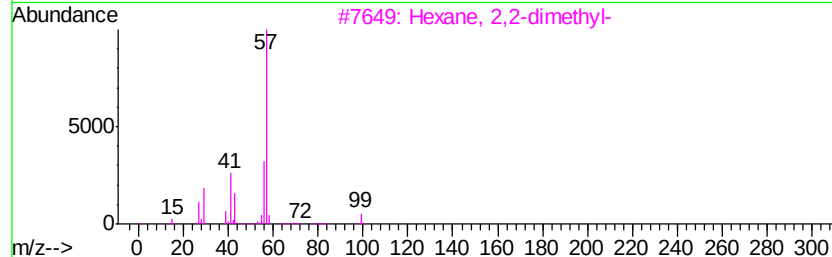
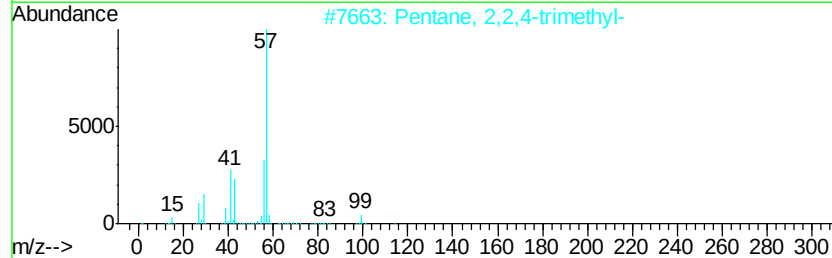
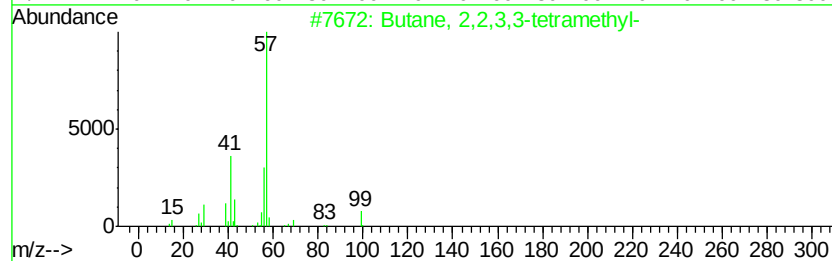
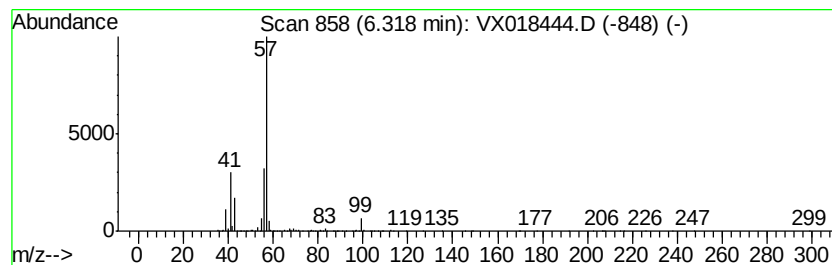
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.32	20.06 ug/l	673071	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
2		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
3		Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	59
4		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45



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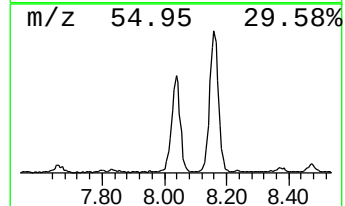
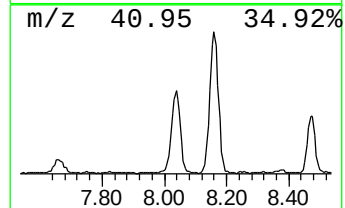
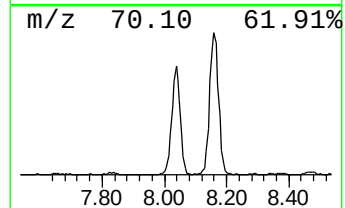
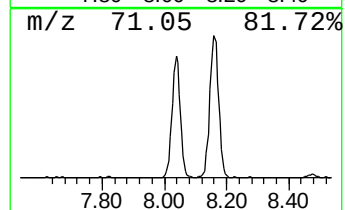
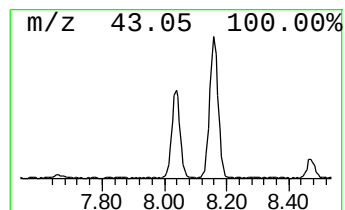
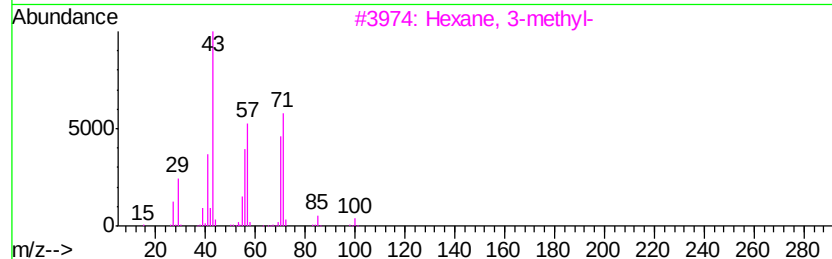
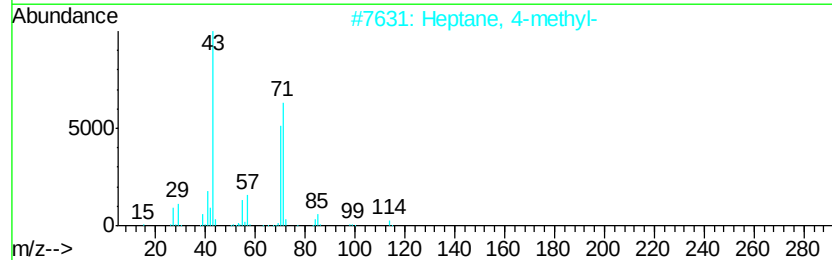
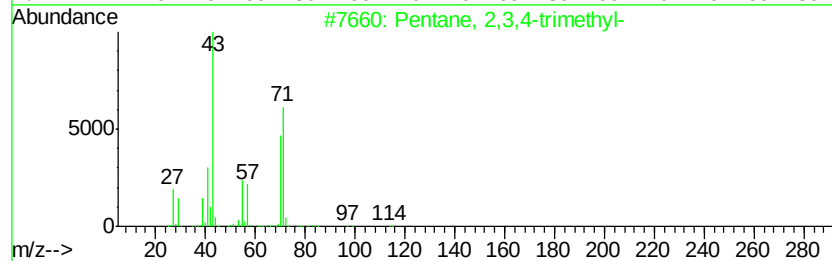
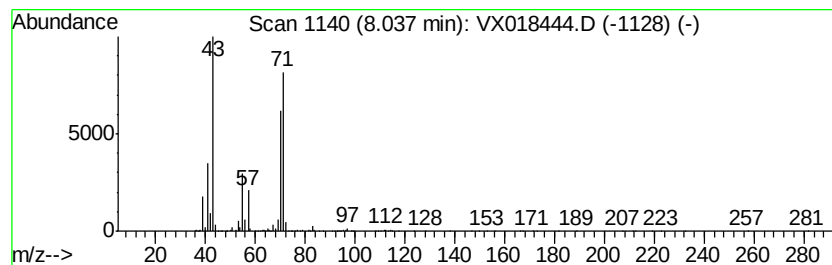
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X082120W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.04	15.16 ug/l	508812	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
4		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78
5		Pentane, 3-ethyl-	100	C7H16	000617-78-7	78



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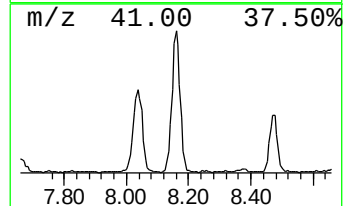
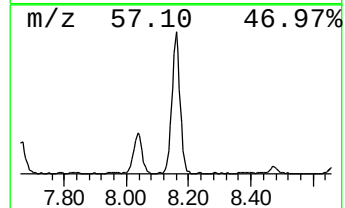
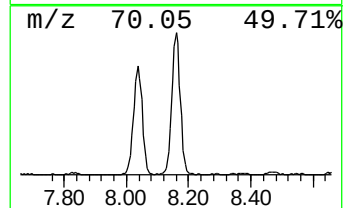
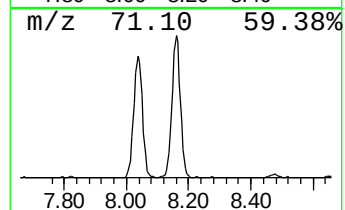
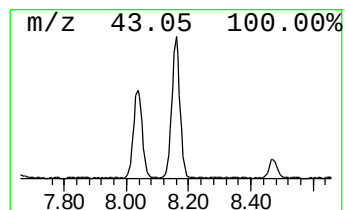
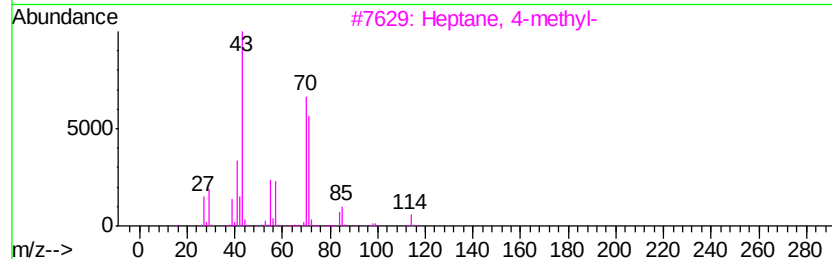
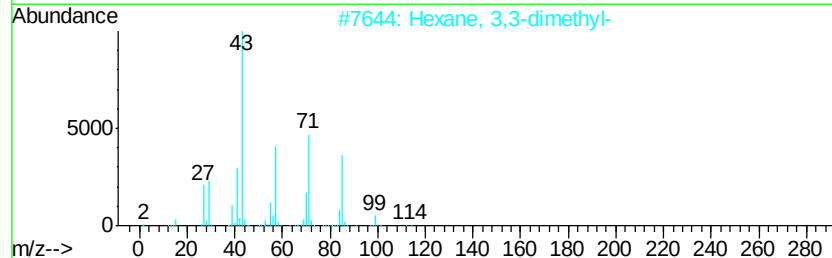
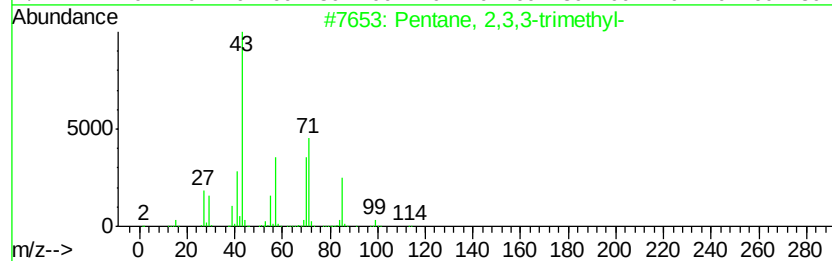
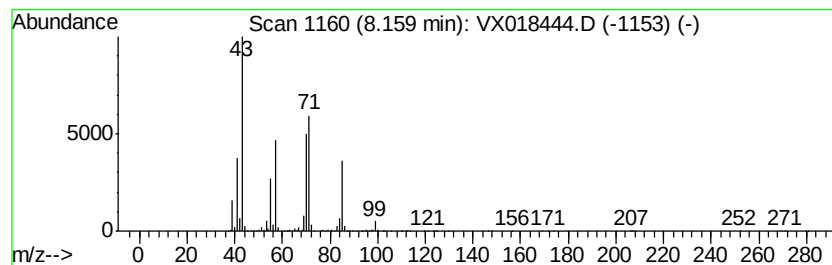
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Quant Title : SW846 8260

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	26.00 ug/l	872350	1,4-Difluorobenzene	6.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	83
2		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	72
3		Heptane, 4-methyl-	114	C8H18	000589-53-7	64
4		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	64



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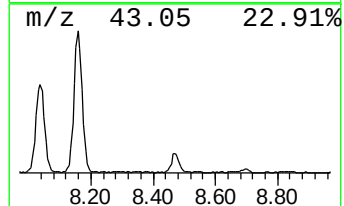
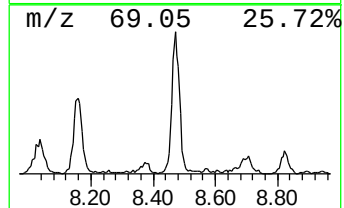
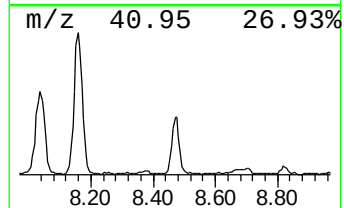
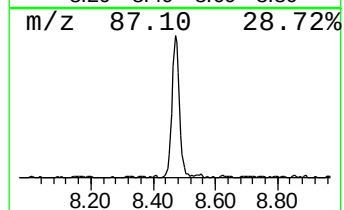
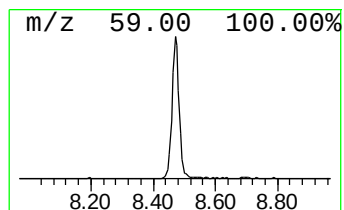
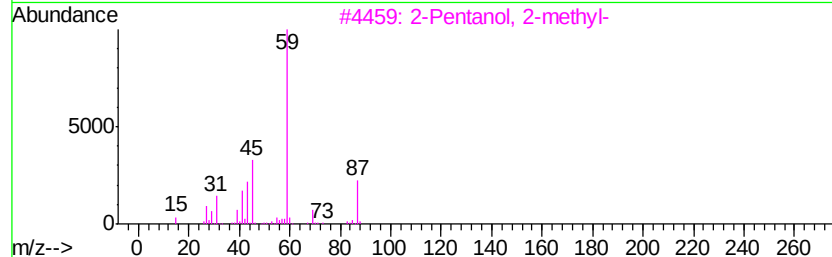
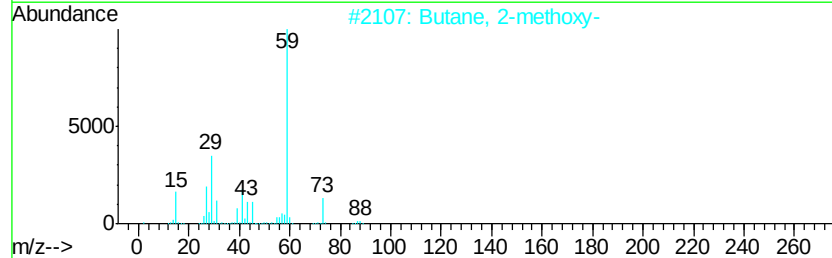
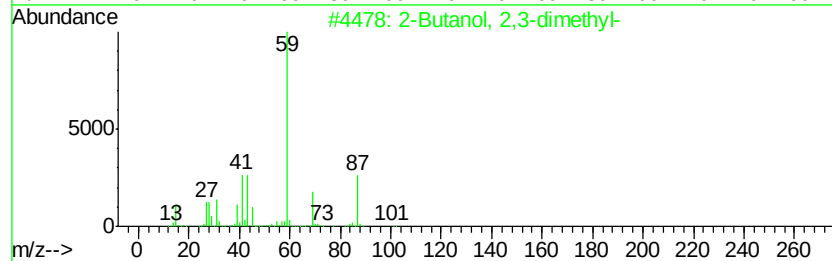
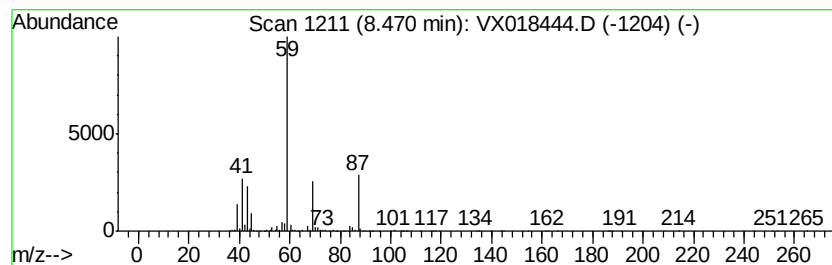
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	5.56 ug/l	266117	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		Butane, 2-methoxy-	88	C5H12O	006795-87-5	64
3		2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	56
4		Pentanamide	101	C5H11NO	000626-97-1	50
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	45



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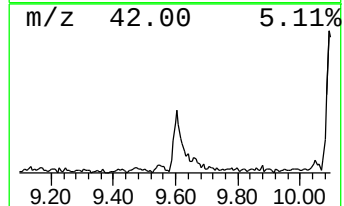
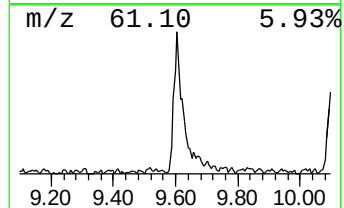
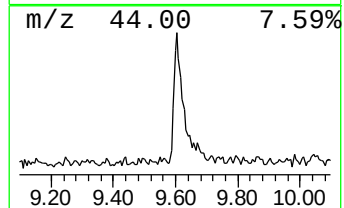
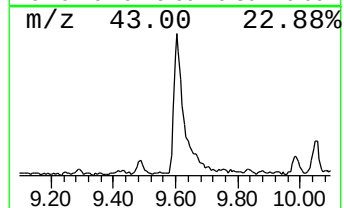
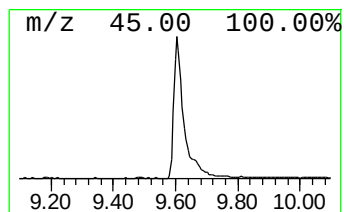
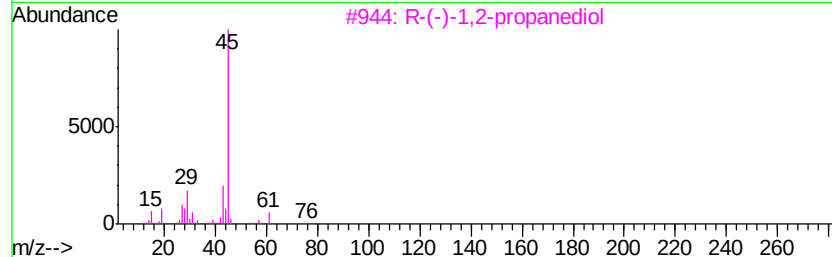
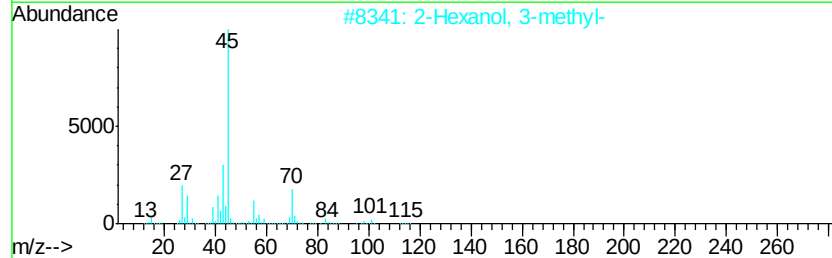
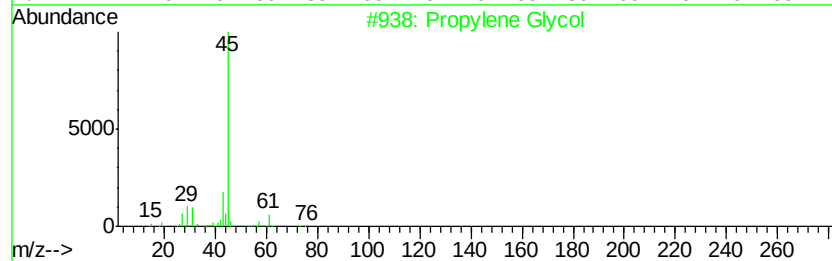
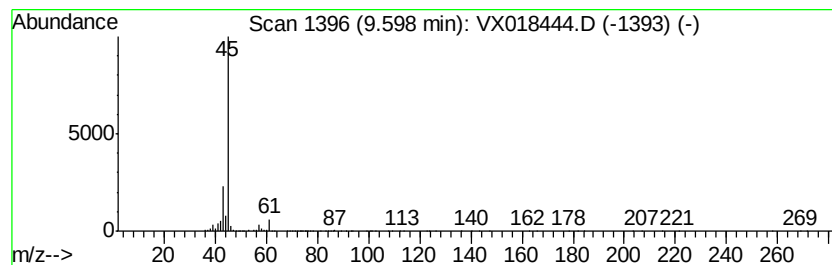
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Propylene Glycol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.60	7.81 ug/l	373784	Chlorobenzene-d5	10.10

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	78
2		2-Hexanol, 3-methyl-	116	C7H16O	002313-65-7	40
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	40
4		2-Pentanol, 4-methyl-	102	C6H14O	000108-11-2	40
5		2-Pentanol	88	C5H12O	006032-29-7	40



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX091620\
Data File : VX018444.D
Acq On : 16 Sep 2020 16:50
Operator : JC/SP
Sample : L3988-27
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FC-DUP06-20200910

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
Butane, 2,2,3,3-t...	6.32	20.1	ug/l	673071	2	6.84	1677710	50.0
Pentane, 2,3,4-tr...	8.04	15.2	ug/l	508812	2	6.84	1677710	50.0
Pentane, 2,3,3-tr...	8.16	26.0	ug/l	872350	2	6.84	1677710	50.0
2-Butanol, 2,3-di...	8.47	5.6	ug/l	266117	3	10.10	2394200	50.0
Propylene Glycol	9.60	7.8	ug/l	373784	3	10.10	2394200	50.0