

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX041819\
 Data File : VX009042.D
 Acq On : 18 Apr 2019 14:34
 Operator : JC/SP
 Sample : K2449-08
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 SS040MW015-190415

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\82X041519W.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	1.617	65	76	79	rBV9	7510	18809	1.44%	0.168%
2	1.788	99	104	110	rBV	15452	24178	1.85%	0.215%
3	2.611	233	239	248	rVB	20300	38244	2.93%	0.341%
4	2.843	269	277	286	rBV	68213	150738	11.54%	1.342%
5	4.306	508	517	530	rBV2	9059	29080	2.23%	0.259%
6	4.574	547	561	562	rBV4	7437	23000	1.76%	0.205%
7	5.501	701	713	727	rBV	133265	379814	29.07%	3.382%
8	5.665	729	740	748	rBV	240644	700283	53.60%	6.236%
9	6.061	795	805	827	rVV	164778	437325	33.47%	3.895%
10	6.348	837	852	868	rVB	385115	1157433	88.59%	10.308%
11	6.860	924	936	949	rBV	390172	917559	70.23%	8.171%
12	7.445	1023	1032	1042	rVB2	21017	49940	3.82%	0.445%
13	7.683	1059	1071	1079	rVB	29212	70041	5.36%	0.624%
14	7.848	1092	1098	1106	rVB2	15881	33551	2.57%	0.299%
15	8.055	1124	1132	1142	rBV	294983	567221	43.42%	5.051%
16	8.177	1143	1152	1161	rVV	469395	902422	69.07%	8.037%
17	8.494	1199	1204	1212	rVB	48485	80142	6.13%	0.714%
18	8.713	1235	1240	1254	rVB	817830	1306441	100.00%	11.635%
19	8.841	1254	1261	1267	rVB	33901	57050	4.37%	0.508%
20	9.043	1289	1294	1301	rVV2	19118	34122	2.61%	0.304%
21	9.165	1305	1314	1319	rBV3	9278	21547	1.65%	0.192%
22	9.256	1326	1329	1332	rVV	9155	14239	1.09%	0.127%
23	9.305	1332	1337	1347	rVB	42119	77820	5.96%	0.693%
24	9.506	1363	1370	1375	rBV2	11820	19833	1.52%	0.177%
25	9.573	1375	1381	1385	rBV3	11429	18073	1.38%	0.161%
26	9.677	1392	1398	1402	rBV	14342	23442	1.79%	0.209%
27	9.890	1428	1433	1441	rVB2	11427	17284	1.32%	0.154%
28	10.110	1464	1469	1475	rBV	734716	1007384	77.11%	8.971%
29	10.335	1501	1506	1515	rVB4	32950	63888	4.89%	0.569%
30	10.433	1515	1522	1528	rBV4	16045	28450	2.18%	0.253%
31	10.512	1531	1535	1544	rVB5	7721	20332	1.56%	0.181%
32	10.609	1544	1551	1555	rBV2	13903	31010	2.37%	0.276%
33	10.658	1555	1559	1564	rVB3	17743	30308	2.32%	0.270%
34	10.798	1577	1582	1586	rBV5	8310	17483	1.34%	0.156%

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35	10.841	1586	1589	1596	rVB3	8417	15443	1.18%	0.138%
36	11.067	1614	1626	1632	rBV	288511	406685	31.13%	3.622%
37	11.134	1632	1637	1642	rVV	577917	757261	57.96%	6.744%
38	11.182	1642	1645	1649	rVB2	18157	24681	1.89%	0.220%
39	11.390	1675	1679	1683	rBV	21767	27219	2.08%	0.242%
40	11.445	1683	1688	1693	rVV5	8743	14783	1.13%	0.132%
41	11.512	1694	1699	1706	rVB2	16142	24366	1.87%	0.217%
42	11.634	1715	1719	1724	rBV	19487	28999	2.22%	0.258%
43	11.768	1733	1741	1745	rBV	45559	67437	5.16%	0.601%
44	11.920	1761	1766	1768	rBV2	10876	14814	1.13%	0.132%
45	11.951	1768	1771	1777	rVV4	9147	18939	1.45%	0.169%
46	12.012	1777	1781	1787	rVV4	14302	28367	2.17%	0.253%
47	12.079	1787	1792	1803	rVB	687421	908652	69.55%	8.092%
48	12.231	1812	1817	1821	rVV	123573	153725	11.77%	1.369%
49	12.292	1821	1827	1831	rVV7	9691	24341	1.86%	0.217%
50	12.341	1831	1835	1837	rVV3	8178	14135	1.08%	0.126%
51	12.377	1837	1841	1849	rVB3	20480	48988	3.75%	0.436%
52	12.719	1891	1897	1900	rVV4	15590	25075	1.92%	0.223%
53	12.755	1900	1903	1909	rVV2	12987	22948	1.76%	0.204%
54	12.816	1909	1913	1916	rVB	16360	19836	1.52%	0.177%
55	12.896	1917	1926	1931	rBV	60596	90216	6.91%	0.803%
56	12.950	1931	1935	1939	rBV2	23899	35860	2.74%	0.319%
57	13.091	1953	1958	1962	rVB	19169	25861	1.98%	0.230%
58	13.249	1979	1984	1989	rVV	21523	26858	2.06%	0.239%
59	13.353	1995	2001	2005	rVB5	8693	14600	1.12%	0.130%
60	13.694	2055	2057	2064	rVB2	12844	20255	1.55%	0.180%

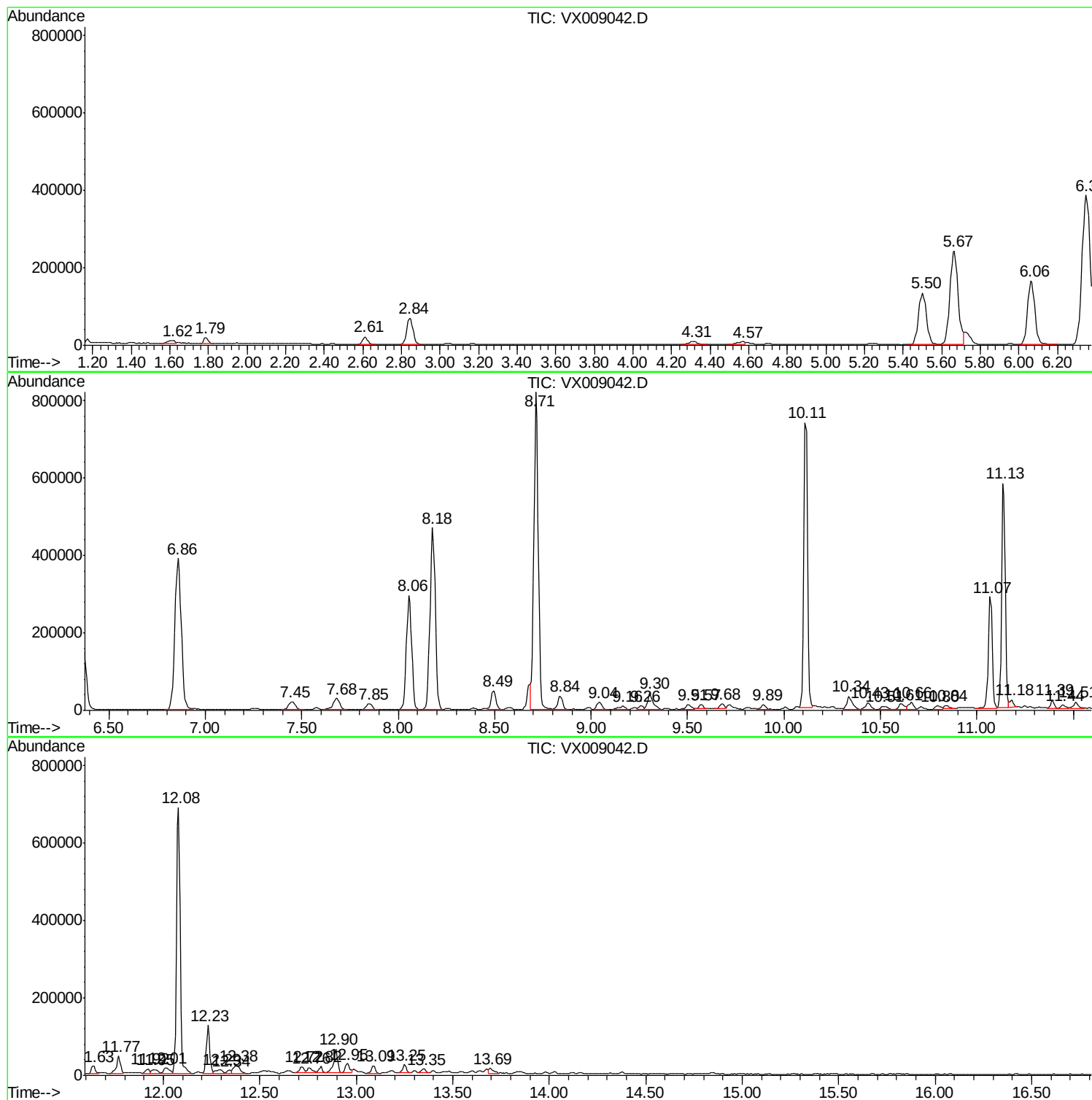
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Quant Title : SW846 8260

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



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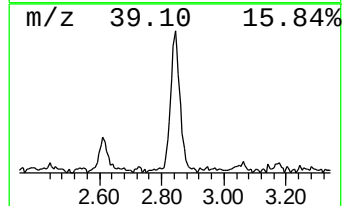
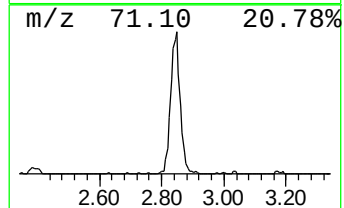
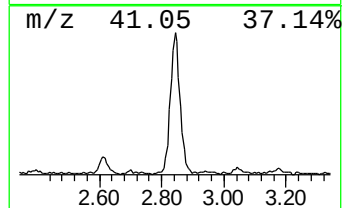
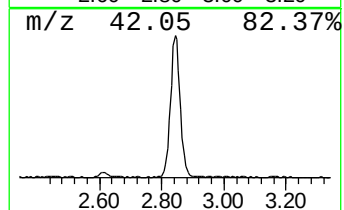
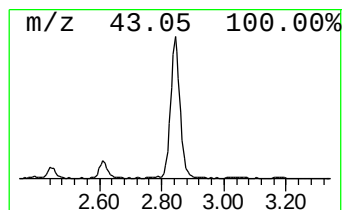
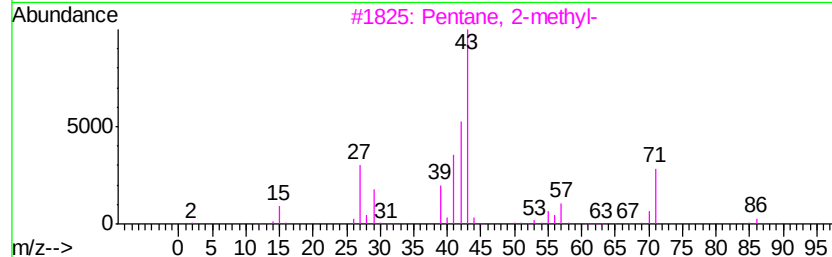
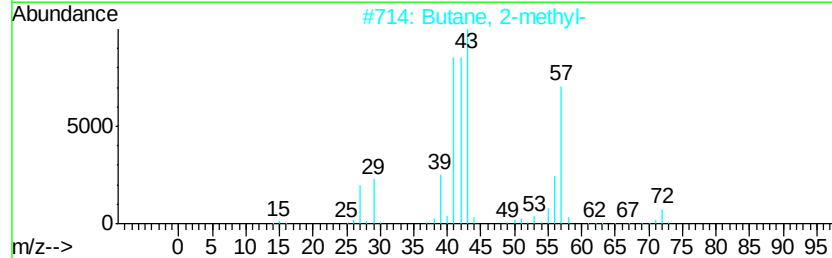
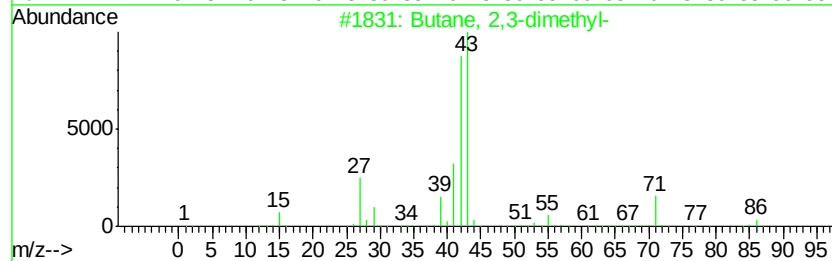
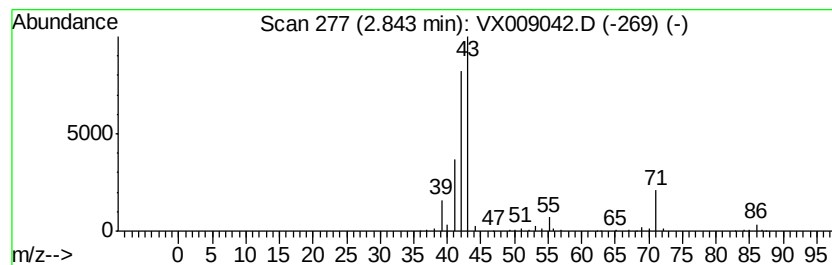
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X041519W.M
Quant Title : SW846 8260

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

Peak Number 1 Butane, 2,3-dimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	10.76 ug/l	150738	Pentafluorobenzene	5.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Butane, 2-methyl-	72	C5H12	000078-78-4	38
3		Pentane, 2-methyl-	86	C6H14	000107-83-5	38
4		Tetrahydrofuran	72	C4H8O	000109-99-9	36
5		Pyrrolidine	71	C4H9N	000123-75-1	10



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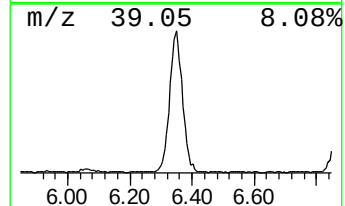
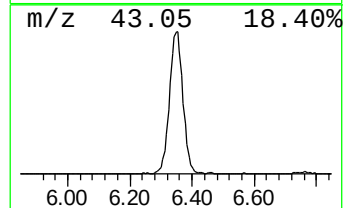
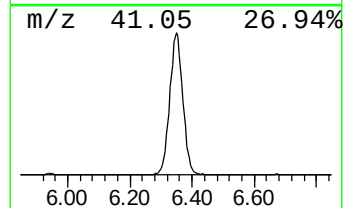
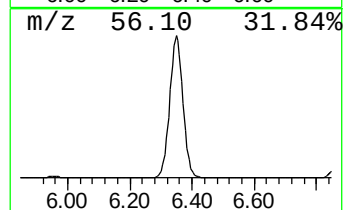
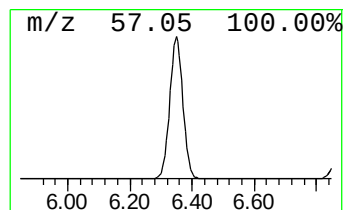
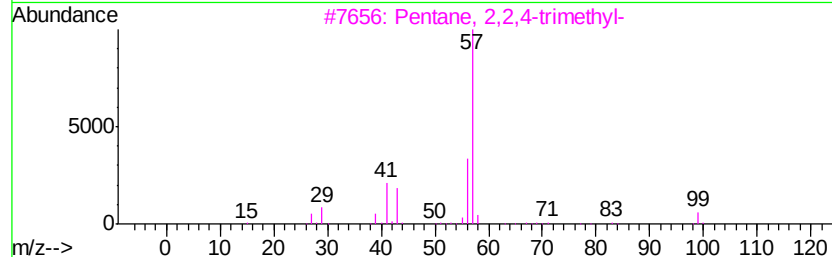
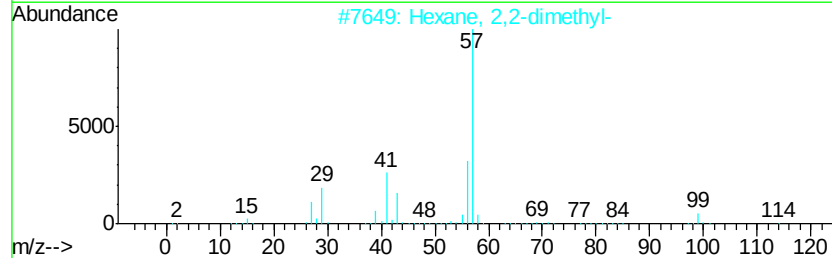
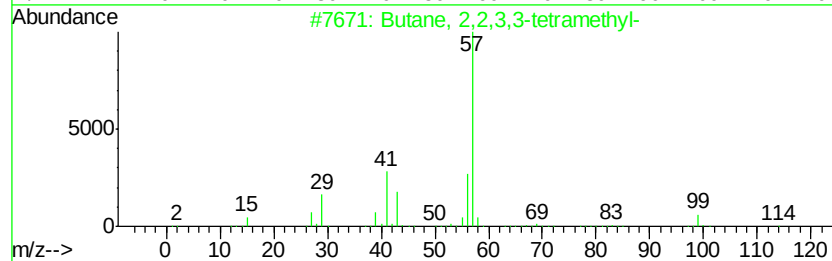
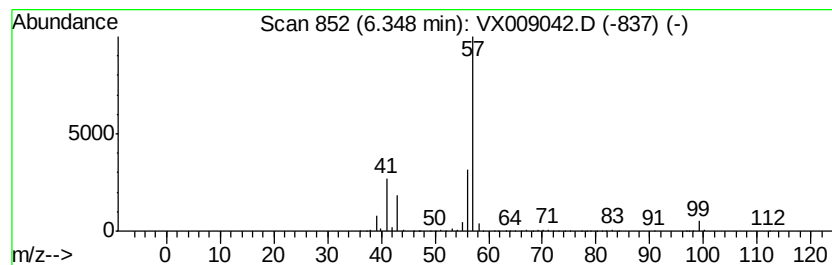
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X041519W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.35	63.07 ug/l	1157430	1,4-Difluorobenzene	6.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	83
2			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	83
3			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	83
4			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	78
5			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64



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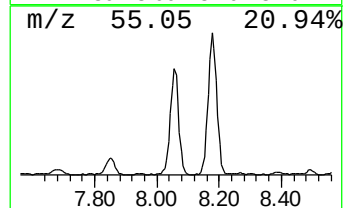
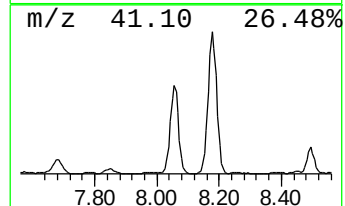
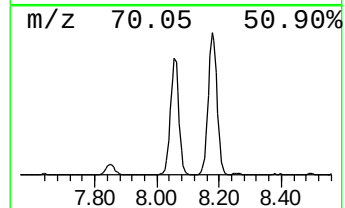
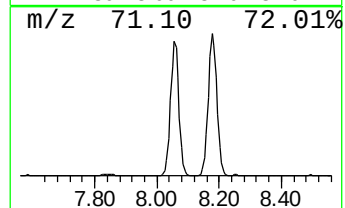
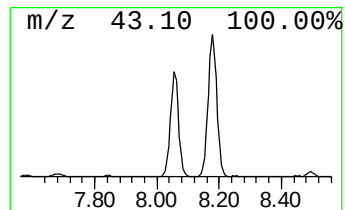
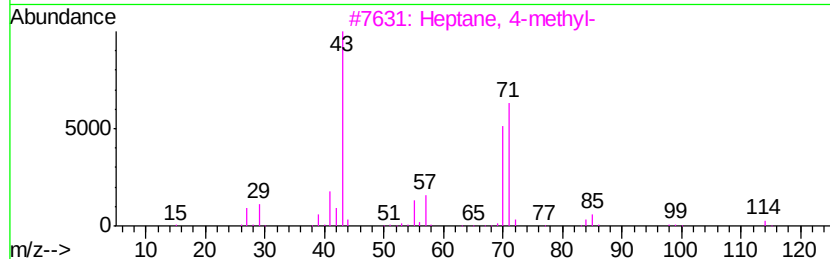
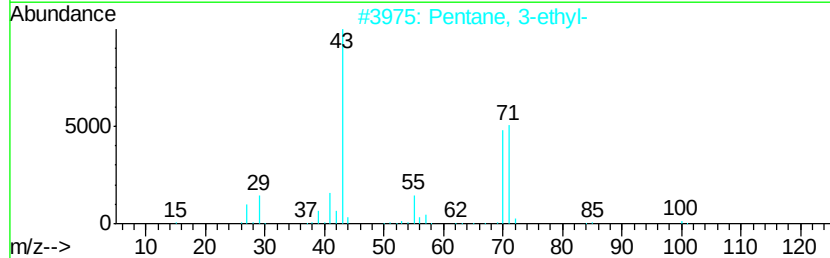
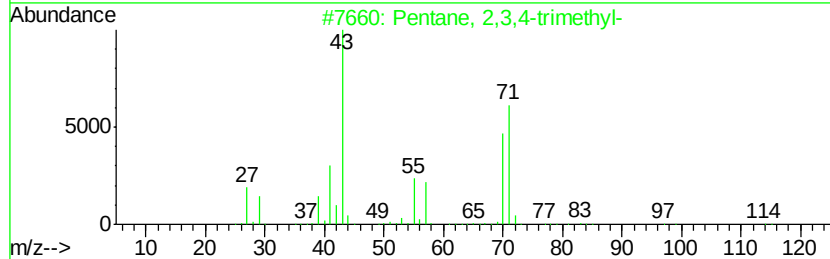
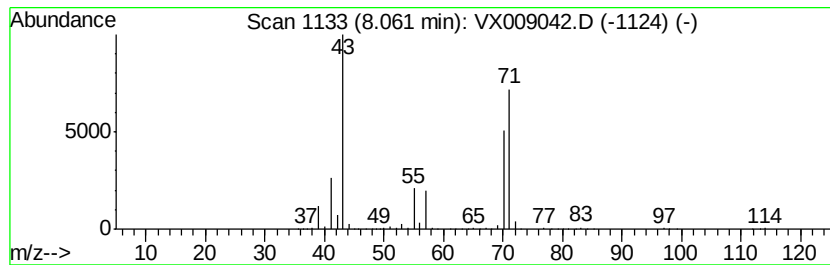
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Pentane, 2,3,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	30.91 ug/l	567221	1,4-Difluorobenzene	6.86
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Pentane, 2,3,4-trimethyl-	114 C8H18	000565-75-3	91
2	Pentane, 3-ethyl-	100 C7H16	000617-78-7	78
3	Heptane, 4-methyl-	114 C8H18	000589-53-7	74
4	Hexane, 3,3,4-trimethyl-	128 C9H20	016747-31-2	72
5	Hexane, 2,3-dimethyl-	114 C8H18	000584-94-1	59



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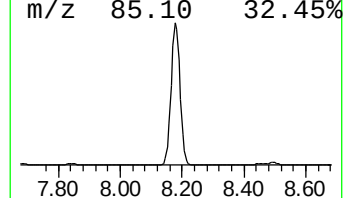
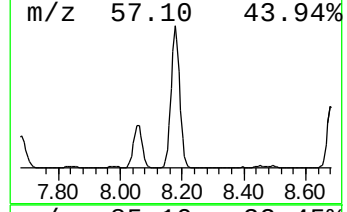
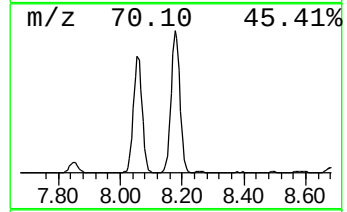
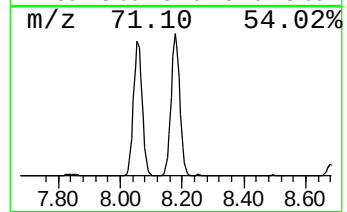
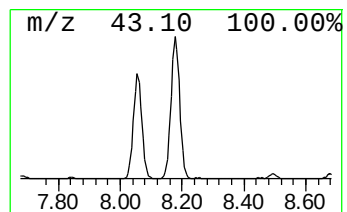
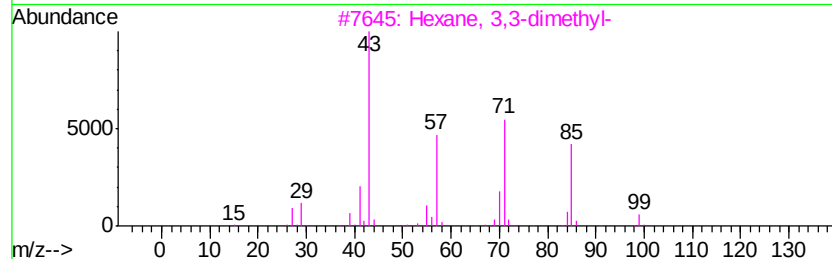
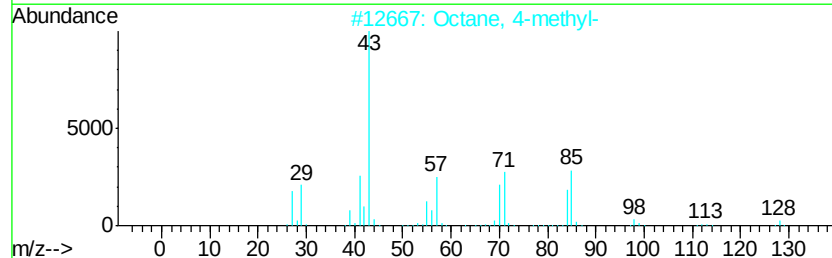
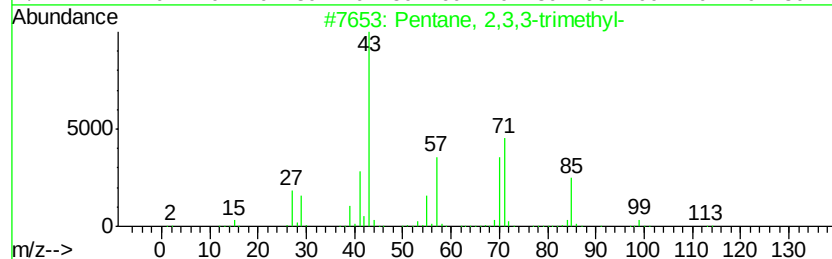
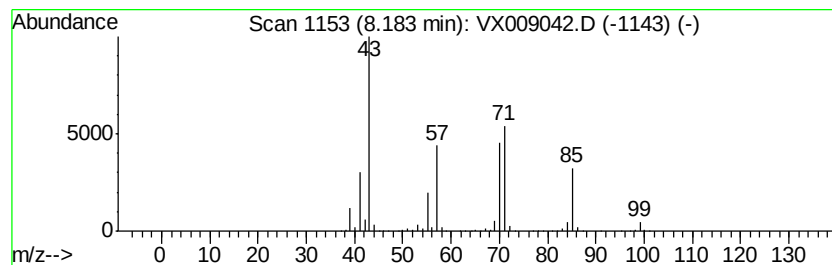
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.18	49.18 ug/l	902422	1,4-Difluorobenzene	6.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Octane, 4-methyl-	128	C9H20	002216-34-4	78
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
5		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59



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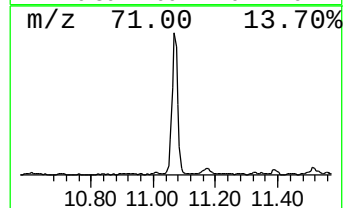
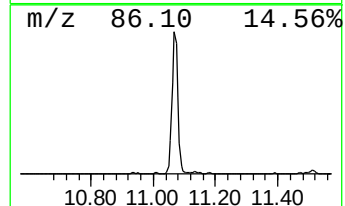
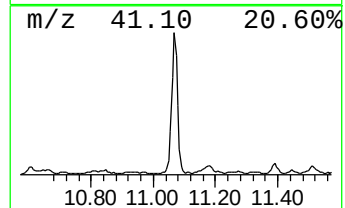
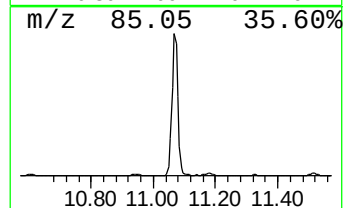
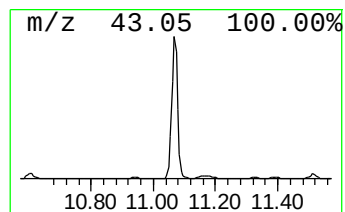
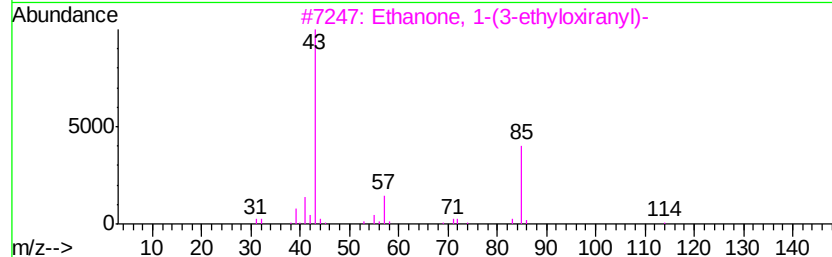
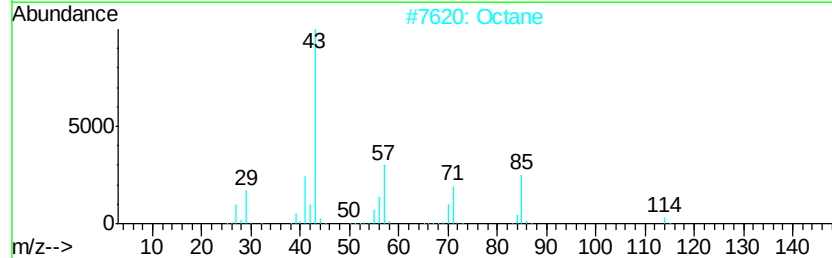
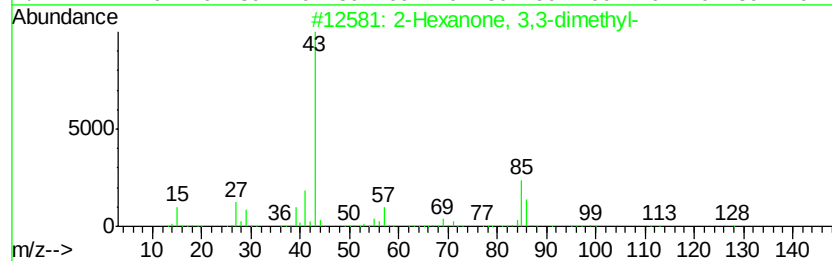
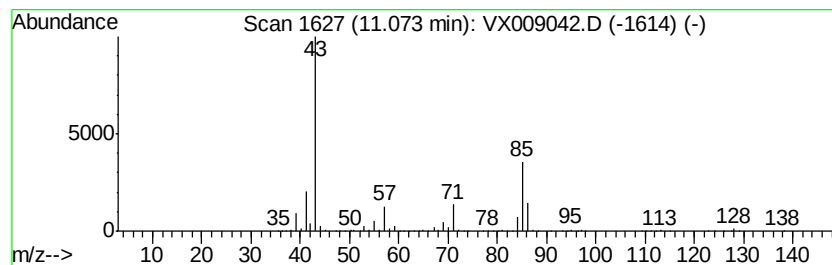
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X041519W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.07	20.19 ug/l	406685	Chlorobenzene-d5	10.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hexanone, 3,3-dimethyl-	128	C8H16O	026118-38-7	72
2		Octane	114	C8H18	000111-65-9	53
3		Ethanone, 1-(3-ethyloxiran-yl)-	114	C6H10O2	017257-81-7	50
4		Hexane, 2-bromo-	164	C6H13Br	003377-86-4	47
5		2-Pentanone, 3-ethyl-3-methyl-	128	C8H16O	019780-65-5	47



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX041819\
Data File : VX009042.D
Acq On : 18 Apr 2019 14:34
Operator : JC/SP
Sample : K2449-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 13 Sample Multiplier: 1

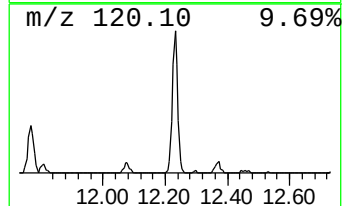
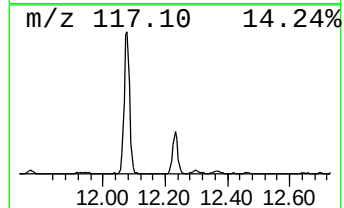
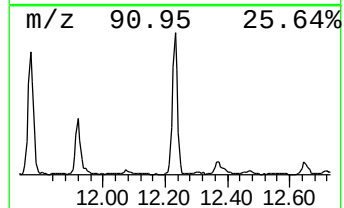
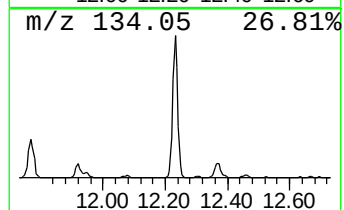
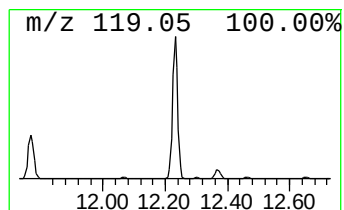
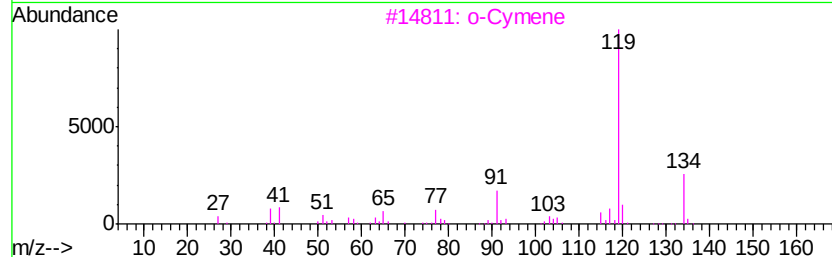
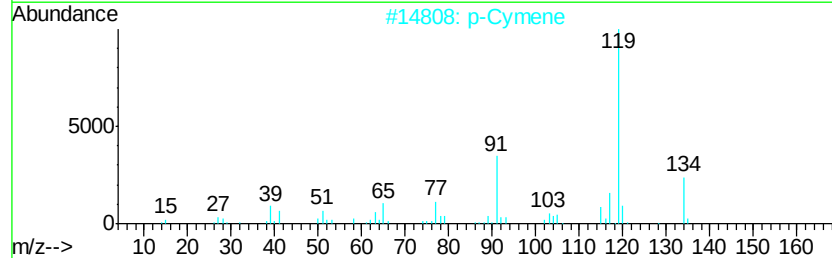
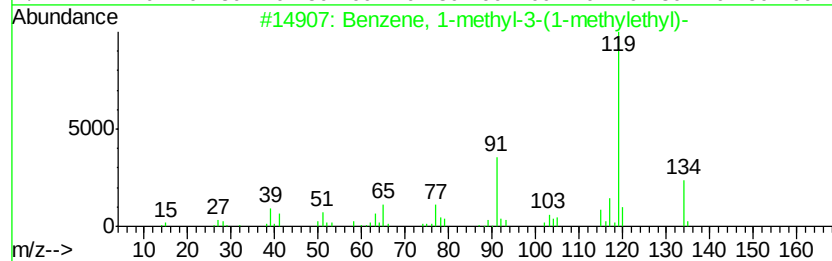
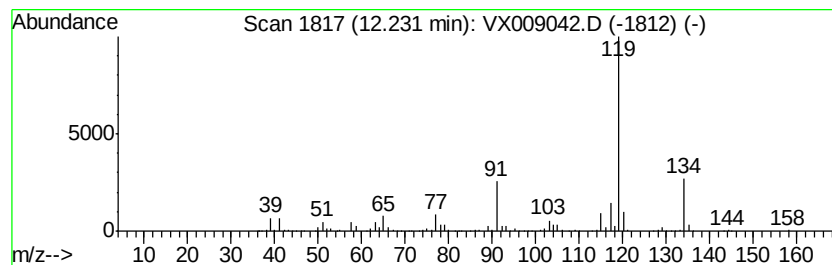
Instrument :
MSVOA_X
ClientSampleId :
SS040MW015-190415

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X041519W.M
Quant Title : SW846 8260

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

Peak Number 6 Benzene, 1-methyl-3-(1-meth... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.23	8.46 ug/l	153725	1,4-Dichlorobenzene-d4	12.08
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Benzene, 1-methyl-3-(1-methyleth...	134 C10H14	000535-77-3	95
2	p-Cymene	134 C10H14	000099-87-6	95
3	o-Cymene	134 C10H14	000527-84-4	94
4	Benzene, 1,2,4,5-tetramethyl-	134 C10H14	000095-93-2	91
5	Benzene, 1,2,3,4-tetramethyl-	134 C10H14	000488-23-3	91



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX041819\
Data File : VX009042.D
Acq On : 18 Apr 2019 14:34
Operator : JC/SP
Sample : K2449-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
SS040MW015-190415

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X041519W.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, 2,3-dimet...	2.84	10.8	ug/l	150738	1	5.67	700283	50.0
Butane, 2,2,3,3-t...	6.35	63.1	ug/l	1157430	2	6.86	917559	50.0
Pentane, 2,3,4-tr...	8.06	30.9	ug/l	567221	2	6.86	917559	50.0
Pentane, 2,3,3-tr...	8.18	49.2	ug/l	902422	2	6.86	917559	50.0
2-Hexanone, 3,3-d...	11.07	20.2	ug/l	406685	3	10.12	1007380	50.0
Benzene, 1-methyl...	12.23	8.5	ug/l	153725	4	12.08	908652	50.0