

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101119\
 Data File : VX013029.D
 Acq On : 11 Oct 2019 20:13
 Operator : JC/SP
 Sample : K5313-08
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA19-JMW3202

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\82X100819W.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	1.070	26	30	40	rBV	978308	1156779	9.37%	1.984%
2	1.393	80	83	89	rBV	459749	466706	3.78%	0.801%
3	1.783	141	147	165	rBV	8728772	12341560	100.00%	21.171%
4	1.991	176	181	195	rVB2	895655	1391626	11.28%	2.387%
5	2.107	195	200	207	rBV	108500	149897	1.21%	0.257%
6	2.259	220	225	234	rVB	86416	140217	1.14%	0.241%
7	2.838	307	320	324	rBV	1516236	3344126	27.10%	5.737%
8	2.881	324	327	347	rVB	704426	1559355	12.63%	2.675%
9	3.161	362	373	390	rBV	467057	1072280	8.69%	1.839%
10	3.515	422	431	443	rBV	243354	548694	4.45%	0.941%
11	4.301	547	560	567	rBV	333526	994664	8.06%	1.706%
12	4.393	567	575	588	rVV	534897	1548465	12.55%	2.656%
13	4.582	588	606	620	rVB3	114315	426102	3.45%	0.731%
14	5.490	744	755	760	rBV2	96795	273930	2.22%	0.470%
15	5.575	760	769	777	rVV2	535902	1831158	14.84%	3.141%
16	5.655	777	782	786	rVV	193851	520271	4.22%	0.893%
17	5.722	786	793	811	rVV	380946	1175034	9.52%	2.016%
18	5.923	814	826	839	rVV4	177902	595817	4.83%	1.022%
19	6.057	839	848	854	rVV	109660	290897	2.36%	0.499%
20	6.136	854	861	871	rVV	206930	545552	4.42%	0.936%
21	6.252	871	880	885	rVV2	119897	349657	2.83%	0.600%
22	6.344	885	895	905	rVV	1275089	3820096	30.95%	6.553%
23	6.447	905	912	925	rVB	162201	450534	3.65%	0.773%
24	6.697	943	953	964	rBV	55893	135969	1.10%	0.233%
25	6.850	969	978	988	rBV	272929	647209	5.24%	1.110%
26	7.459	1065	1078	1089	rBV	770549	1794874	14.54%	3.079%
27	7.569	1089	1096	1101	rVV	123308	254082	2.06%	0.436%
28	7.636	1101	1107	1111	rVV	162462	364384	2.95%	0.625%
29	7.673	1111	1113	1118	rVV	89069	161816	1.31%	0.278%
30	7.728	1118	1122	1133	rVV2	106255	202138	1.64%	0.347%
31	8.051	1164	1175	1184	rBV	774274	1559637	12.64%	2.675%
32	8.173	1186	1195	1203	rBV	1097872	2156315	17.47%	3.699%
33	8.252	1203	1208	1213	rVB	164935	271180	2.20%	0.465%
34	8.666	1268	1276	1279	rBV3	236461	484405	3.92%	0.831%

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Integration Parameters: RTEINT.P

Integrator: RTE
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35	8.709	1279	1283	1289	rVV	587082	959295	7.77%	1.646%
36	8.782	1289	1295	1299	rVV	226220	340863	2.76%	0.585%
37	8.837	1299	1304	1308	rVB	87557	135918	1.10%	0.233%
38	9.038	1331	1337	1344	rVB	162173	263729	2.14%	0.452%
39	9.160	1348	1357	1363	rBV	87025	148621	1.20%	0.255%
40	9.617	1428	1432	1437	rVV	157918	220369	1.79%	0.378%
41	9.672	1437	1441	1446	rVV	101371	150616	1.22%	0.258%
42	10.111	1507	1513	1519	rBV	513175	706549	5.72%	1.212%
43	10.245	1529	1535	1544	rVB	693268	936235	7.59%	1.606%
44	10.355	1544	1553	1559	rBV	1711721	2345466	19.00%	4.024%
45	10.696	1605	1609	1620	rVB	110480	153167	1.24%	0.263%
46	11.014	1656	1661	1666	rBV	271601	343262	2.78%	0.589%
47	11.135	1675	1681	1685	rBV	405128	526599	4.27%	0.903%
48	11.355	1711	1717	1724	rBV	312497	384163	3.11%	0.659%
49	11.428	1724	1729	1731	rBV	428186	571472	4.63%	0.980%
50	11.501	1737	1741	1749	rVB	524860	629895	5.10%	1.081%
51	11.666	1762	1768	1776	rBV	466243	584007	4.73%	1.002%
52	11.806	1786	1791	1801	rVB	1171473	1512207	12.25%	2.594%
53	12.019	1818	1826	1830	rBV	141511	174420	1.41%	0.299%
54	12.074	1830	1835	1840	rVV2	532420	721481	5.85%	1.238%
55	12.135	1840	1845	1851	rVB	369283	469205	3.80%	0.805%
56	12.300	1865	1872	1873	rBV2	186852	243856	1.98%	0.418%
57	12.318	1873	1875	1879	rVV	175491	206131	1.67%	0.354%
58	12.367	1879	1883	1892	rVB3	214940	339092	2.75%	0.582%
59	12.513	1902	1907	1914	rBV	157502	187386	1.52%	0.321%
60	12.580	1914	1918	1920	rBV	108950	138492	1.12%	0.238%
61	12.605	1920	1922	1927	rVB	118220	126373	1.02%	0.217%
62	12.666	1927	1932	1935	rBV	140956	173067	1.40%	0.297%
63	12.757	1942	1947	1954	rBV3	137242	276577	2.24%	0.474%
64	12.897	1965	1970	1975	rVB2	95523	128204	1.04%	0.220%
65	12.970	1975	1982	1986	rVV	100551	149054	1.21%	0.256%
66	13.013	1986	1989	1995	rVB	163582	195336	1.58%	0.335%
67	13.342	2039	2043	2048	rBV2	173677	241173	1.95%	0.414%
68	13.830	2115	2123	2130	rVB	105027	160016	1.30%	0.275%
69	14.690	2251	2264	2268	rBV	158190	230313	1.87%	0.395%
70	14.836	2283	2288	2297	rBV	144805	195397	1.58%	0.335%

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Integration Parameters: RTEINT.P
Integrator: RTE
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Title : SW846 8260

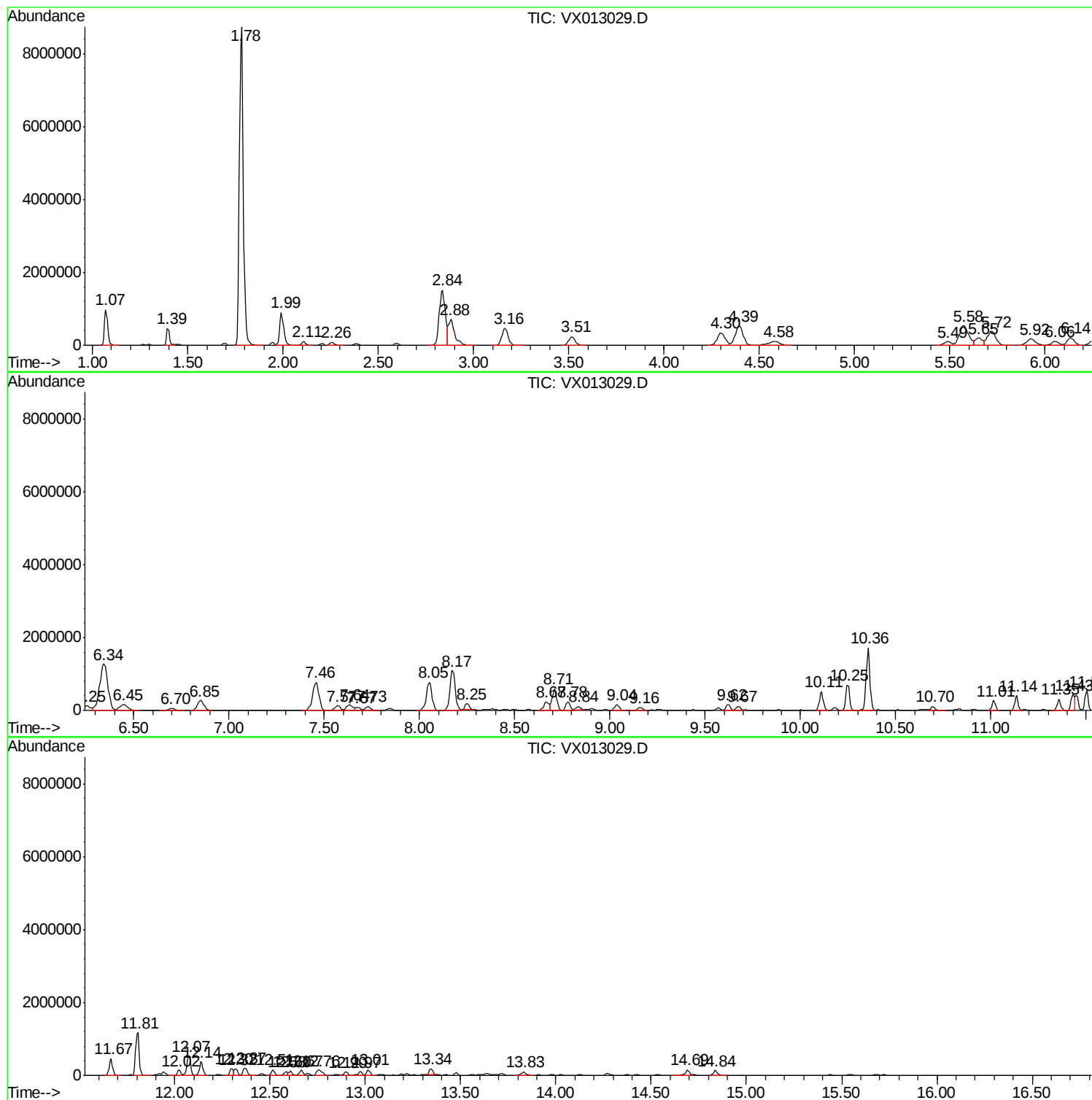
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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



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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

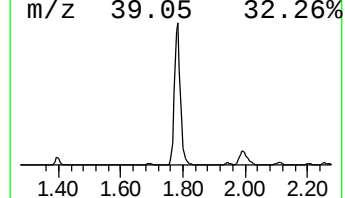
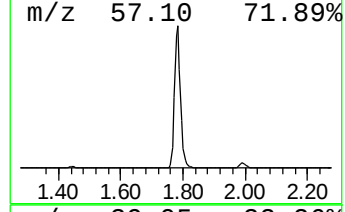
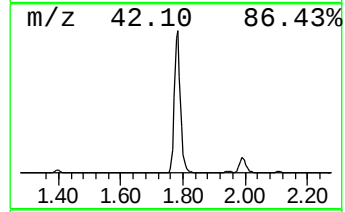
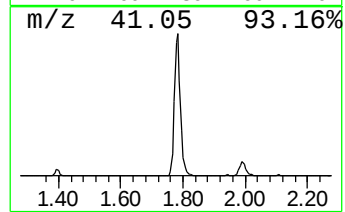
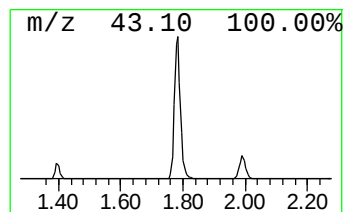
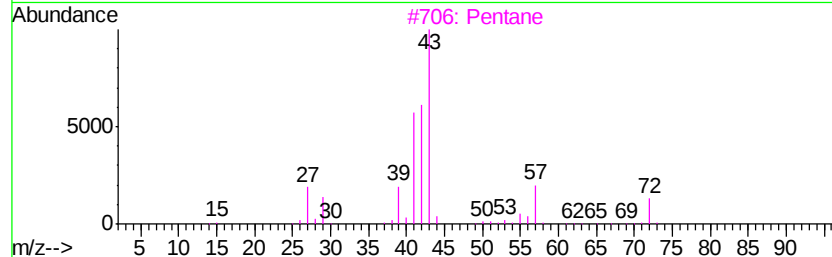
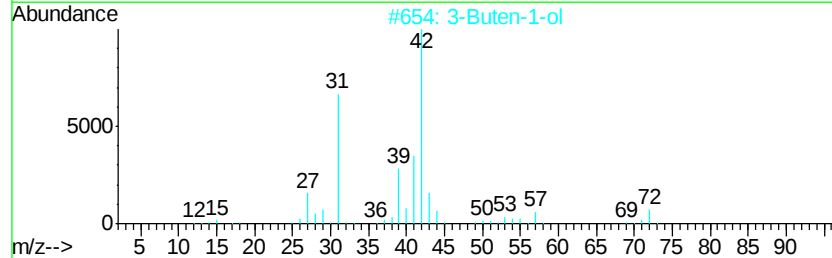
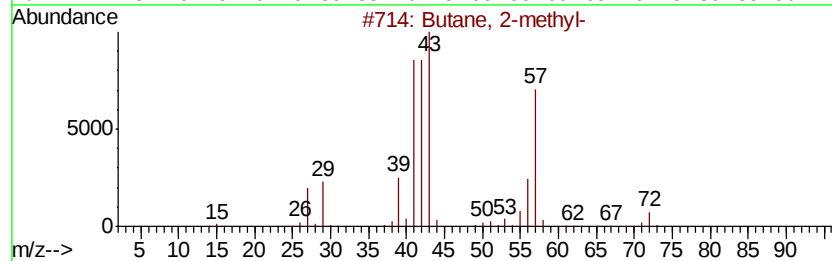
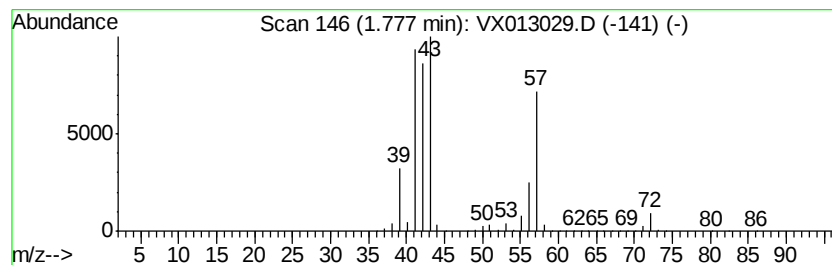
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	1186.07 ug/l	12341600	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methyl-	72	C5H12	000078-78-4	94
2		3-Buten-1-ol	72	C4H8O	000627-27-0	47
3		Pentane	72	C5H12	000109-66-0	33
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5		Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10



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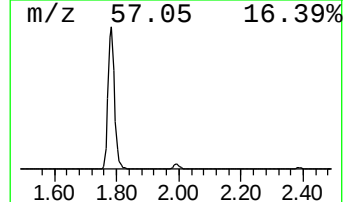
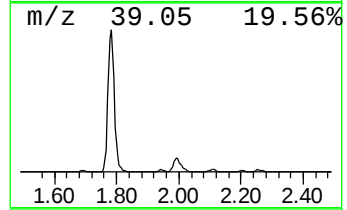
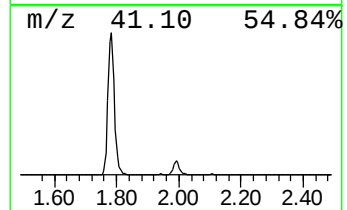
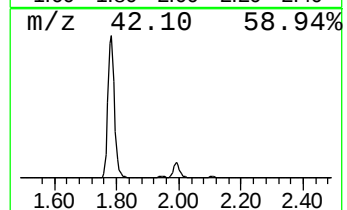
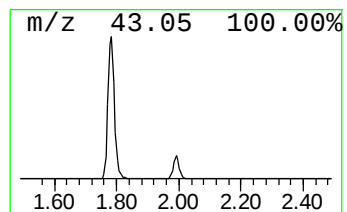
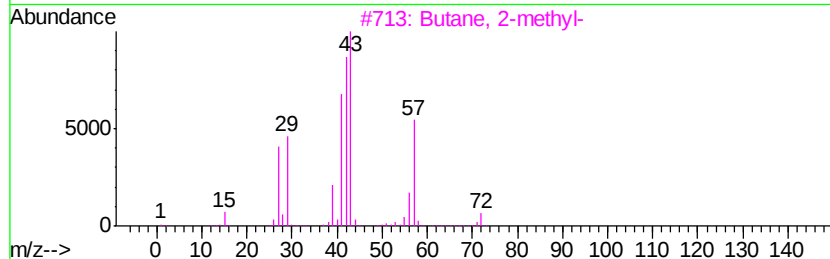
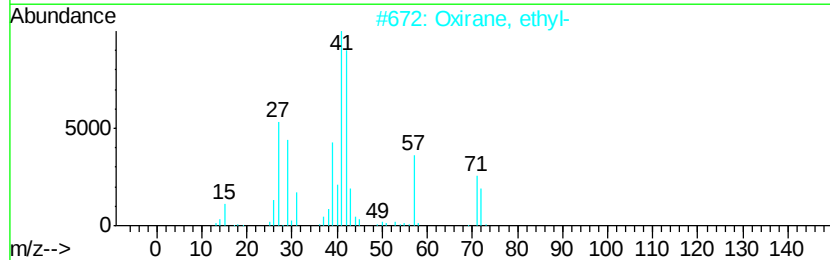
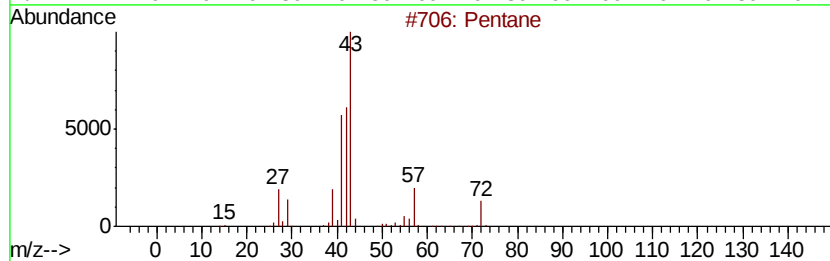
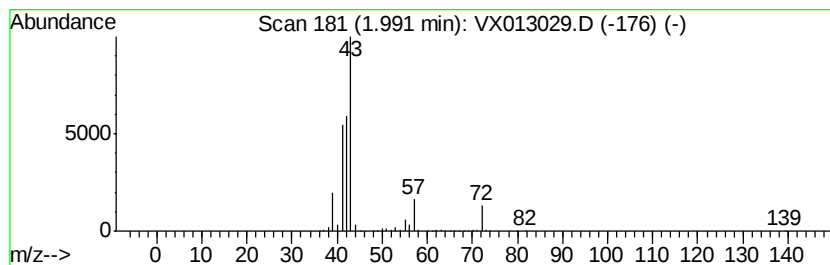
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 3 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	133.74 ug/l	1391630	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane	72	C5H12	000109-66-0	91
2		Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3		Butane, 2-methyl-	72	C5H12	000078-78-4	38
4		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5		Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9



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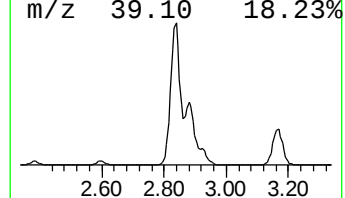
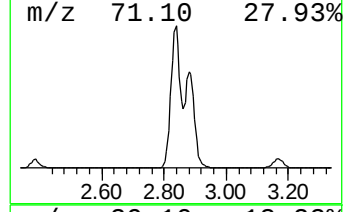
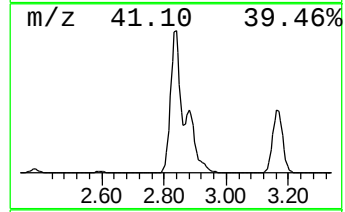
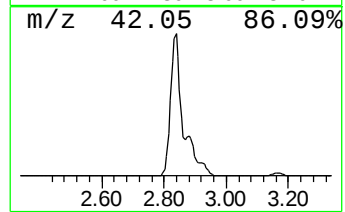
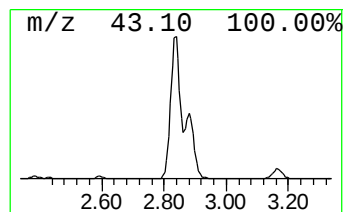
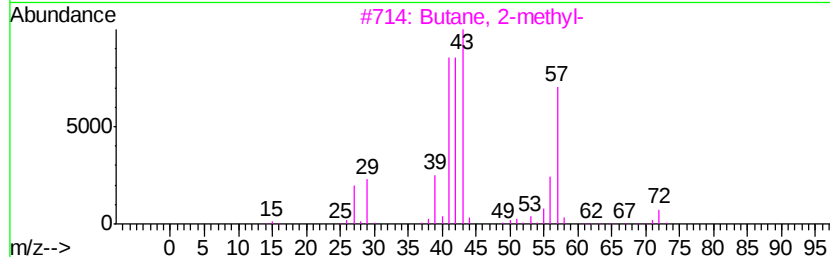
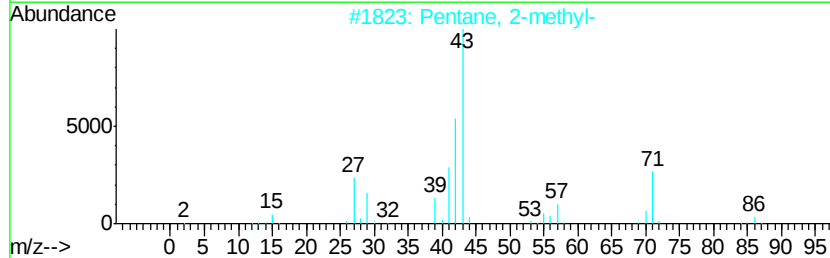
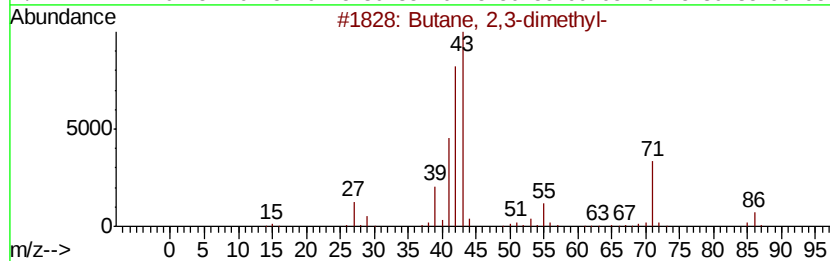
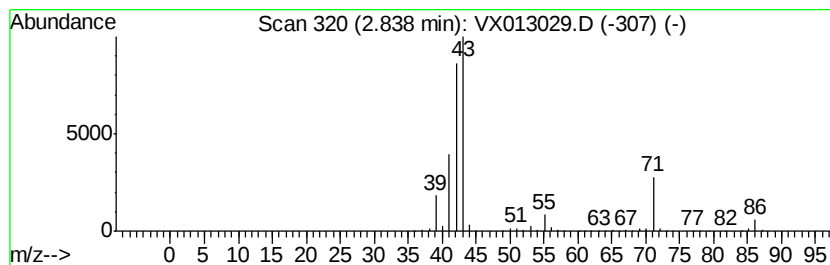
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	321.38 ug/l	3344130	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3		Butane, 2-methyl-	72	C5H12	000078-78-4	36
4		Pyrrolidine	71	C4H9N	000123-75-1	22
5		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	12



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MSVOA_X
ClientSampled :
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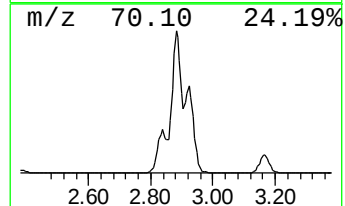
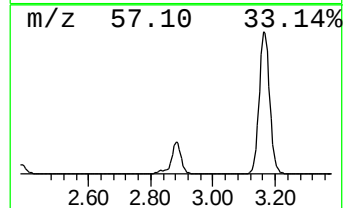
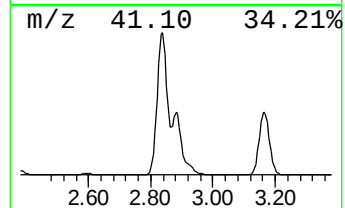
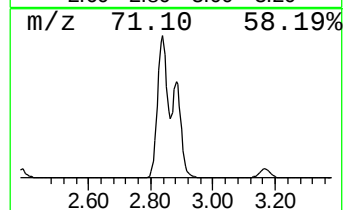
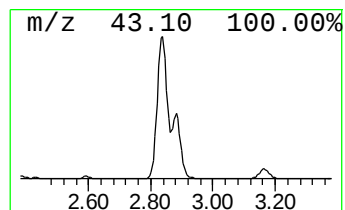
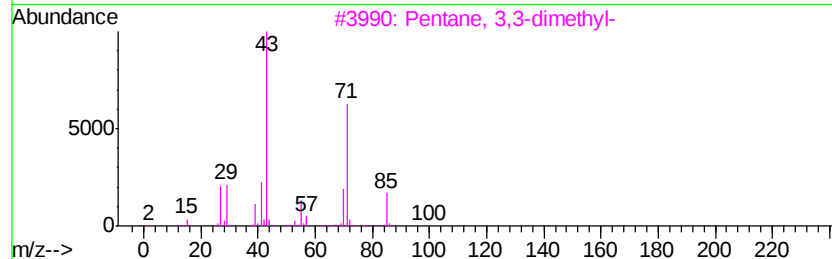
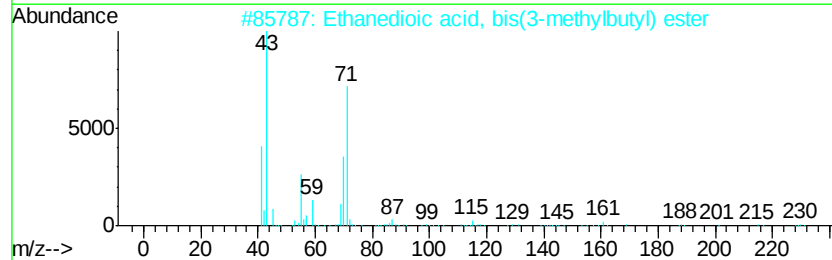
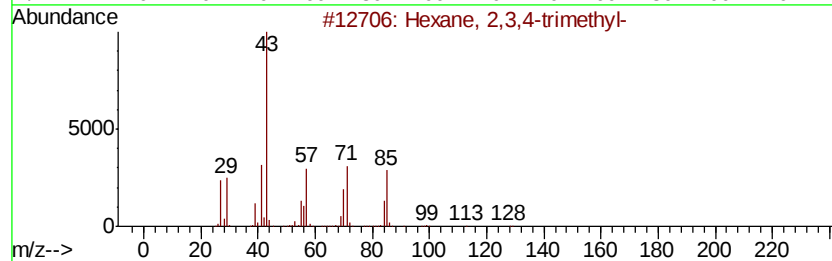
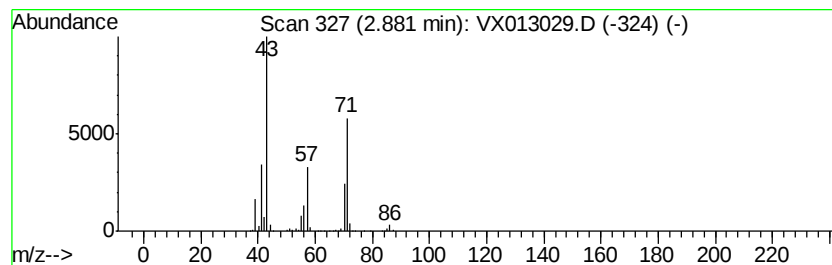
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 5 Hexane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	149.86 ug/l	1559360	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	59
2		Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	56
3		Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	56
4		Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	40
5		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

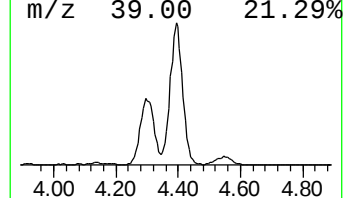
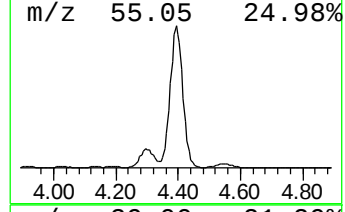
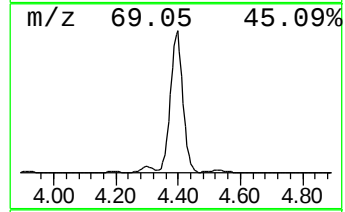
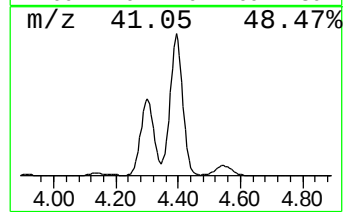
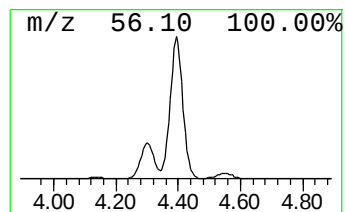
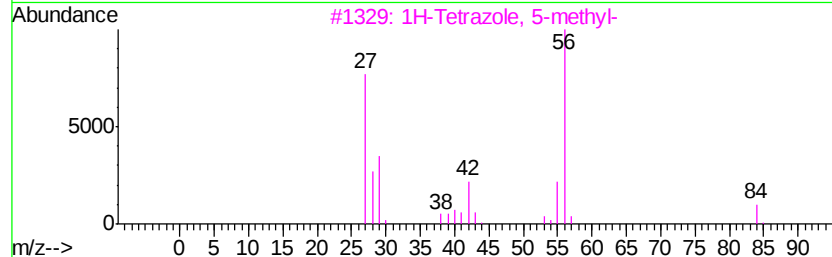
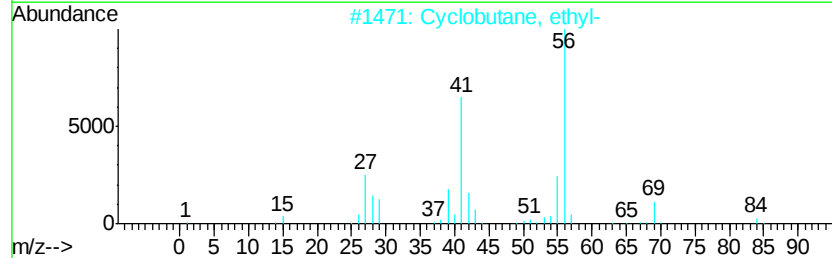
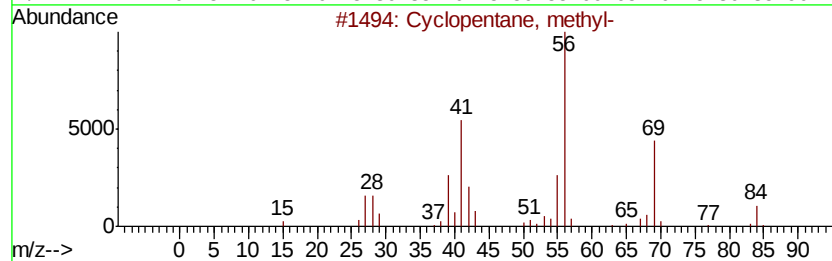
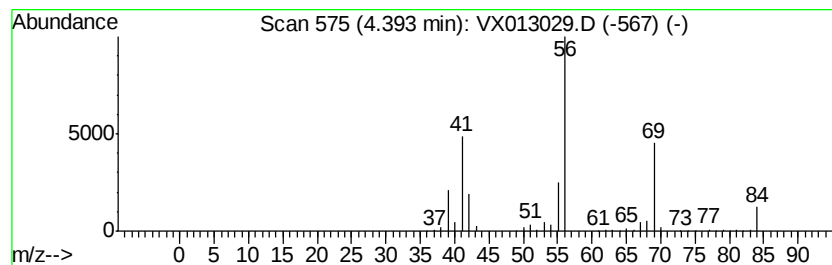
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	148.81 ug/l	1548470	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	56
5		1-Octene, 7-methyl-	126	C9H18	013151-06-9	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

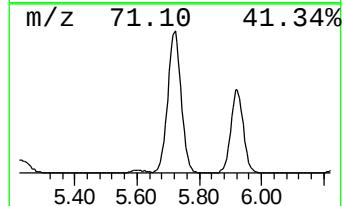
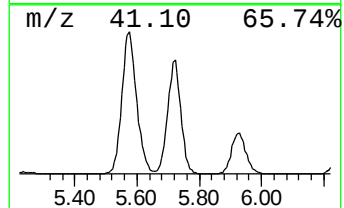
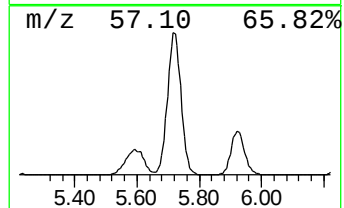
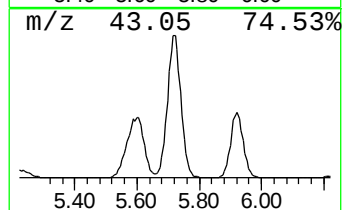
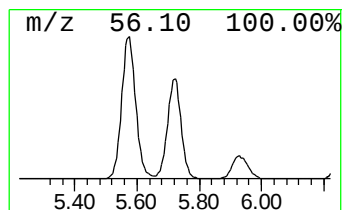
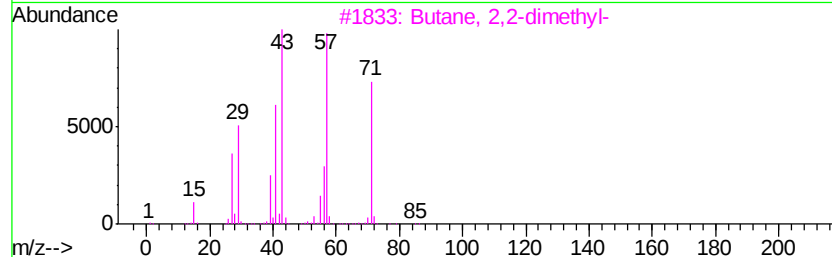
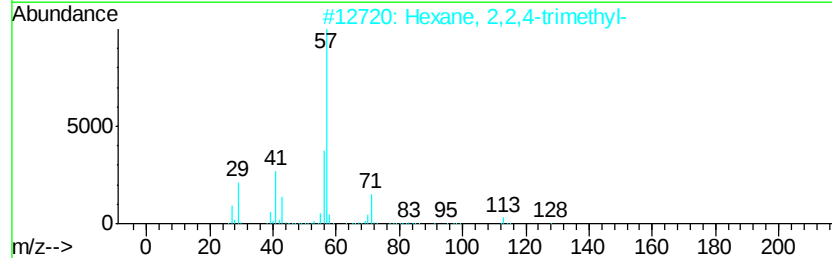
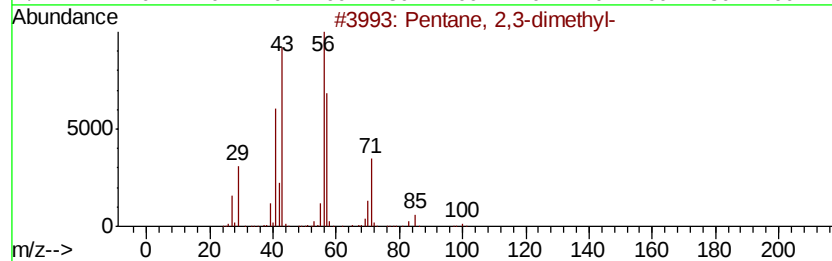
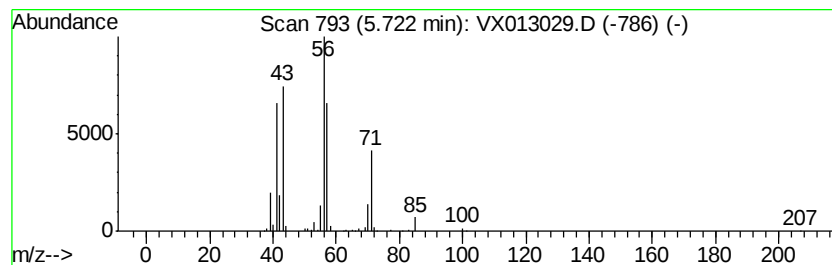
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Quant Title : SW846 8260

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

Peak Number 7 Pentane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	112.93 ug/l	1175030	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3-dimethyl-	100	C7H16	000565-59-3	91
2		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	45
3		Butane, 2,2-dimethyl-	86	C6H14	000075-83-2	38
4		Heptane	100	C7H16	000142-82-5	37
5		1-Hexene, 2-methyl-	98	C7H14	006094-02-6	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

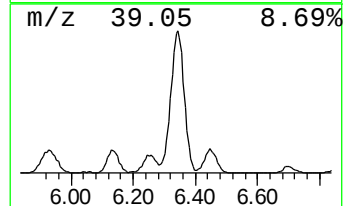
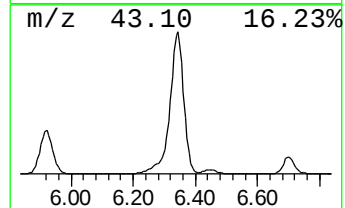
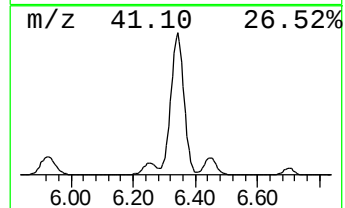
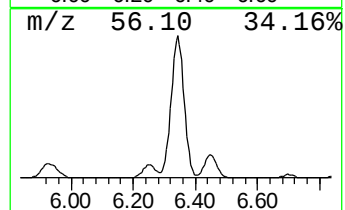
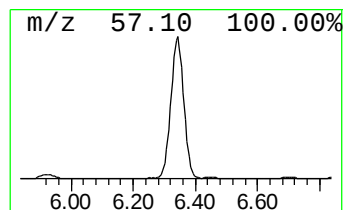
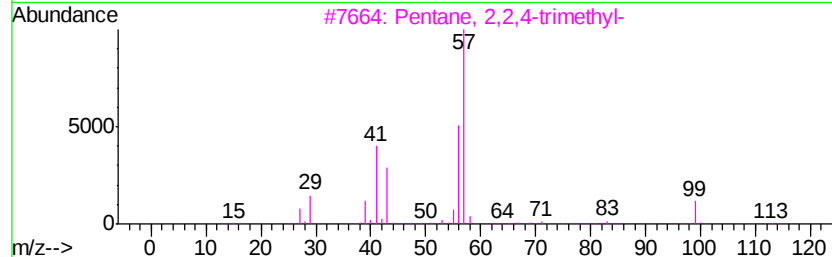
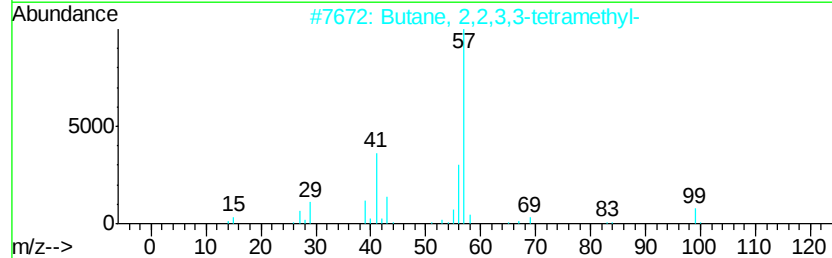
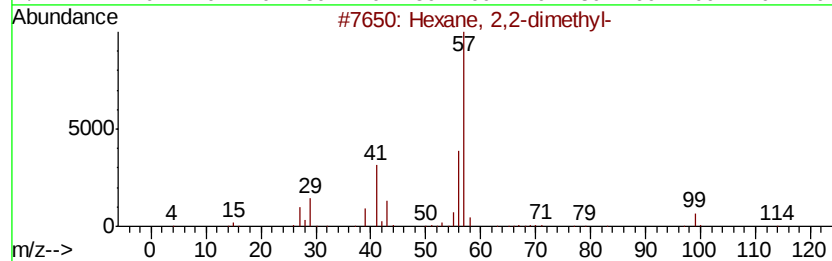
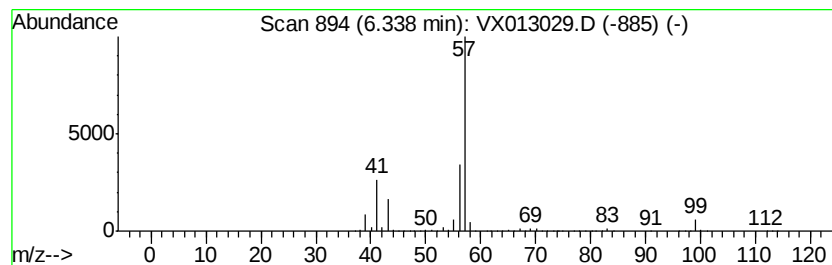
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Quant Title : SW846 8260

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

Peak Number 8 Hexane, 2,2-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	295.12 ug/l	3820100	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
2		Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3		Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5		Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

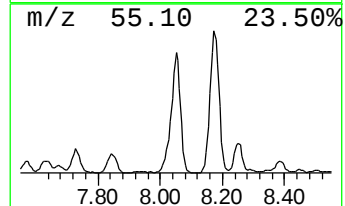
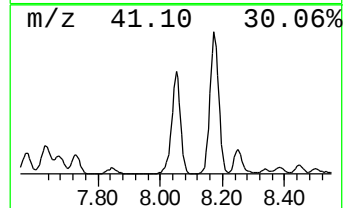
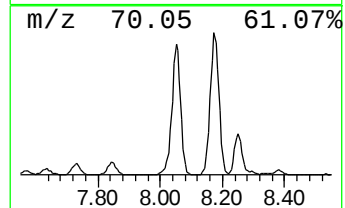
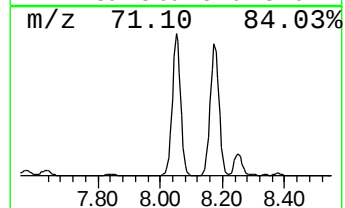
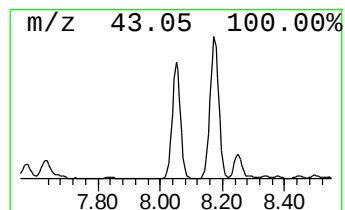
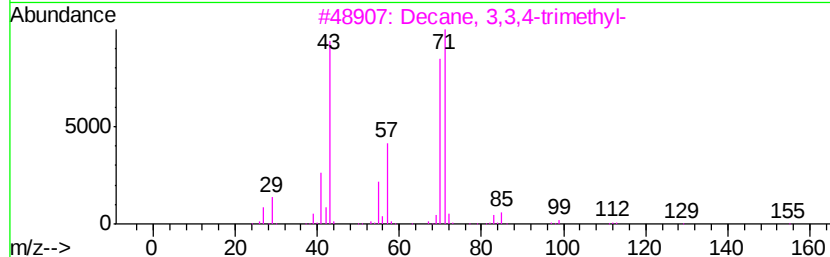
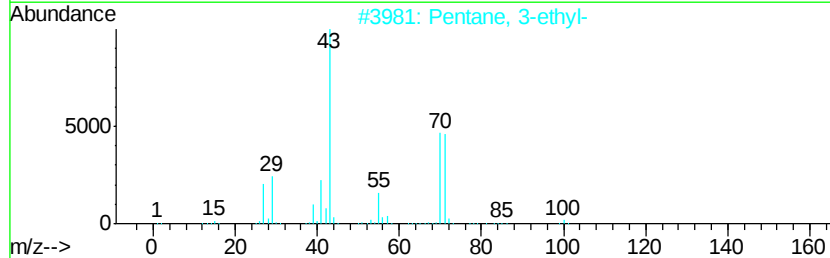
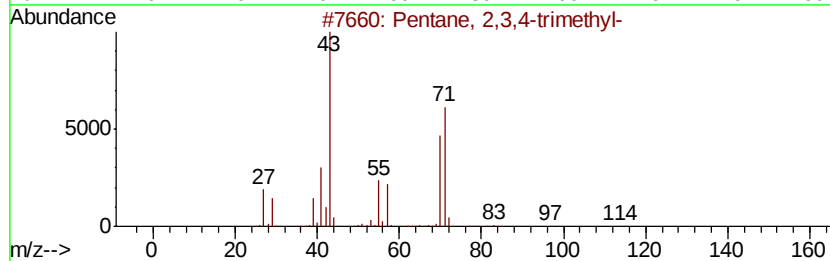
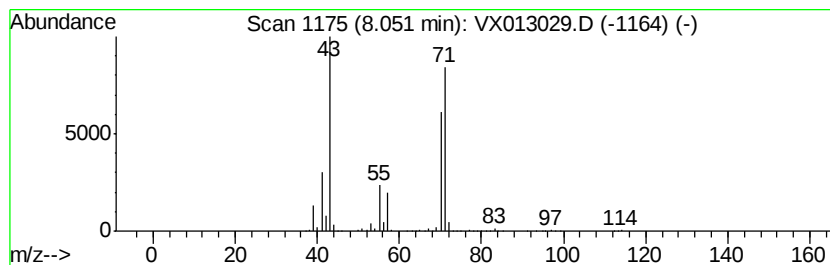
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Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,4-trimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	120.49 ug/l	1559640	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	91
2		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
3		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74
4		2,4,4-Trimethyl-1-hexene	126	C9H18	051174-12-0	64
5		Heptane, 3,3,4-trimethyl-	142	C10H22	020278-87-9	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
FA19-JMW3202

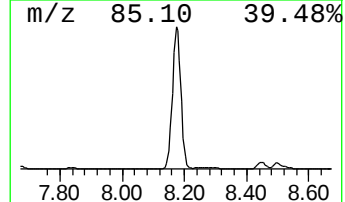
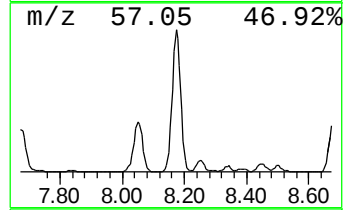
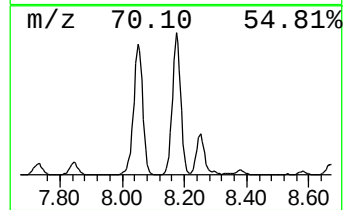
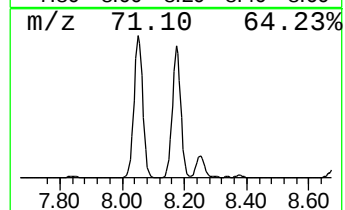
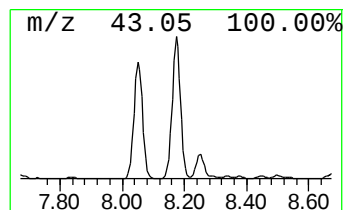
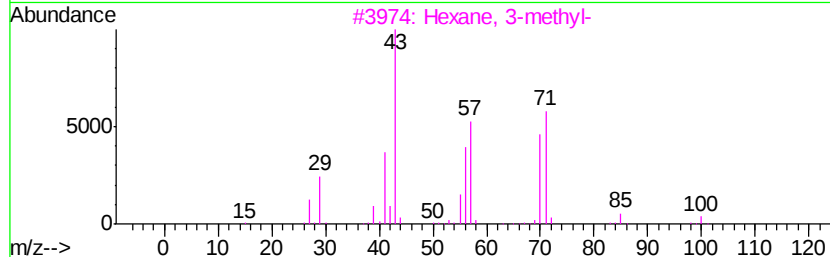
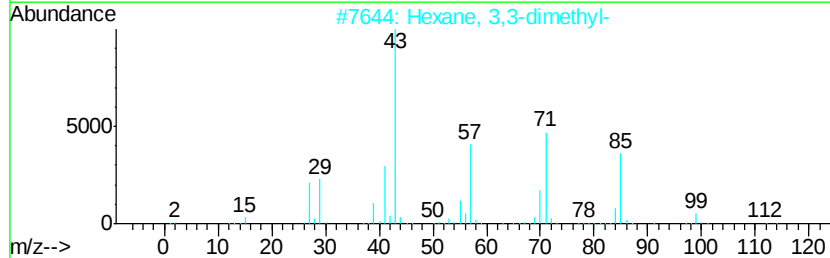
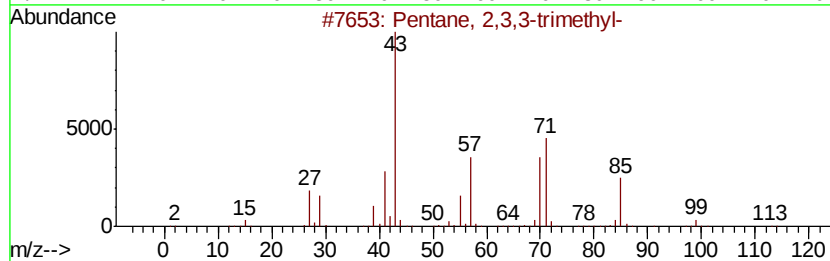
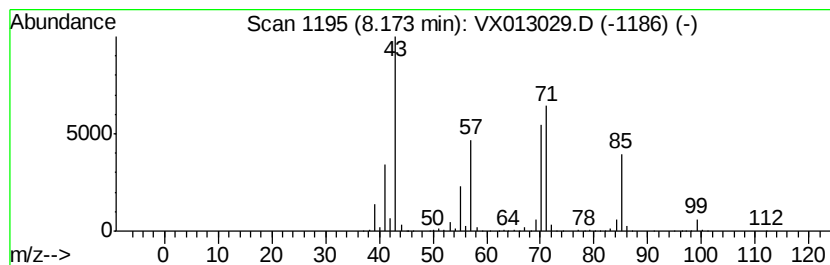
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Quant Title : SW846 8260

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

Peak Number 10 Pentane, 2,3,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	166.59 ug/l	2156320	1,4-Difluorobenzene	6.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
3			Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4			Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	50
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101119\
Data File : VX013029.D
Acq On : 11 Oct 2019 20:13
Operator : JC/SP
Sample : K5313-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JMW3202

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.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-methyl-	1.78	1186.1	ug/l	12341600	1	5.65	520271	50.0
Pentane	1.99	133.7	ug/l	1391630	1	5.65	520271	50.0
Butane, 2,3-dimet...	2.84	321.4	ug/l	3344130	1	5.65	520271	50.0
Hexane, 2,3,4-tri...	2.88	149.9	ug/l	1559360	1	5.65	520271	50.0
Cyclopentane, met...	4.39	148.8	ug/l	1548470	1	5.65	520271	50.0
Pentane, 2,3-dime...	5.72	112.9	ug/l	1175030	1	5.65	520271	50.0
Hexane, 2,2-dimet...	6.34	295.1	ug/l	3820100	2	6.85	647209	50.0
Pentane, 2,3,4-tr...	8.05	120.5	ug/l	1559640	2	6.85	647209	50.0
Pentane, 2,3,3-tr...	8.17	166.6	ug/l	2156320	2	6.85	647209	50.0