

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101419\
 Data File : VX013059.D
 Acq On : 14 Oct 2019 18:03
 Operator : JC/SP
 Sample : K5313-04
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA19-JBW7333

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	41	rBV	699469	848160	8.84%	1.939%
2	1.393	80	83	89	rBV	311030	326145	3.40%	0.745%
3	1.783	141	147	168	rVV	6897033	9599703	100.00%	21.941%
4	1.991	177	181	194	rVB2	548387	840744	8.76%	1.922%
5	2.838	300	320	325	rBV	1298749	2998186	31.23%	6.853%
6	2.881	325	327	344	rVB	528368	1034818	10.78%	2.365%
7	3.167	365	374	390	rVB	379350	871649	9.08%	1.992%
8	3.515	422	431	445	rBV	126767	288659	3.01%	0.660%
9	4.301	547	560	568	rBV	273070	834768	8.70%	1.908%
10	4.393	568	575	589	rVB	325522	939001	9.78%	2.146%
11	4.582	589	606	616	rBV3	58714	249296	2.60%	0.570%
12	5.490	739	755	760	rBV	97126	270526	2.82%	0.618%
13	5.575	760	769	776	rVV2	319300	1069474	11.14%	2.444%
14	5.649	776	781	786	rVV	187884	538903	5.61%	1.232%
15	5.722	786	793	808	rVB	313903	977841	10.19%	2.235%
16	5.929	814	827	839	rBV5	124788	423735	4.41%	0.968%
17	6.057	839	848	854	rVV	111708	292843	3.05%	0.669%
18	6.136	854	861	871	rVV	166608	433404	4.51%	0.991%
19	6.252	871	880	885	rVV2	95835	283899	2.96%	0.649%
20	6.344	885	895	905	rVV	1225287	3673474	38.27%	8.396%
21	6.447	905	912	925	rVB2	121252	339347	3.53%	0.776%
22	6.850	968	978	990	rBV	274960	652477	6.80%	1.491%
23	7.459	1064	1078	1089	rBV2	444726	1073328	11.18%	2.453%
24	7.569	1089	1096	1101	rVV	113938	234116	2.44%	0.535%
25	7.630	1101	1106	1111	rVV	156743	350613	3.65%	0.801%
26	7.679	1111	1114	1118	rVV	86585	154005	1.60%	0.352%
27	7.728	1118	1122	1133	rVV	77479	148418	1.55%	0.339%
28	8.051	1164	1175	1186	rVB	737843	1479834	15.42%	3.382%
29	8.173	1186	1195	1203	rBV	1066115	2060545	21.46%	4.710%
30	8.252	1203	1208	1219	rVB	138141	254233	2.65%	0.581%
31	8.666	1268	1276	1279	rBV3	199758	413974	4.31%	0.946%
32	8.709	1279	1283	1290	rVB	573073	922567	9.61%	2.109%
33	8.837	1299	1304	1308	rBV	73334	116011	1.21%	0.265%
34	9.038	1331	1337	1344	rVB	124883	202445	2.11%	0.463%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON
Sampling : 1
Start Thrs: 0.2
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35	9.160	1348	1357	1363	rBV	68872	116981	1.22%	0.267%
36	9.617	1428	1432	1437	rVV	123910	169604	1.77%	0.388%
37	9.672	1437	1441	1446	rVV	81242	118876	1.24%	0.272%
38	10.111	1507	1513	1519	rBV	513685	702973	7.32%	1.607%
39	10.245	1530	1535	1544	rVB	414415	555693	5.79%	1.270%
40	10.355	1544	1553	1560	rBV	909703	1275544	13.29%	2.915%
41	11.014	1656	1661	1672	rBV	187697	240118	2.50%	0.549%
42	11.135	1675	1681	1685	rBV	387547	507983	5.29%	1.161%
43	11.355	1709	1717	1724	rBV	196466	243756	2.54%	0.557%
44	11.428	1724	1729	1731	rBV	233131	311050	3.24%	0.711%
45	11.501	1737	1741	1749	rVB	249834	298066	3.10%	0.681%
46	11.666	1762	1768	1776	rBV	262464	340730	3.55%	0.779%
47	11.800	1786	1790	1802	rVB	606567	773571	8.06%	1.768%
48	12.019	1819	1826	1830	rVV	93118	120518	1.26%	0.275%
49	12.074	1830	1835	1841	rVV2	515950	695984	7.25%	1.591%
50	12.135	1841	1845	1855	rVB	168505	220039	2.29%	0.503%
51	12.300	1865	1872	1873	rBV	123894	161203	1.68%	0.368%
52	12.318	1873	1875	1879	rVV	130367	148515	1.55%	0.339%
53	12.367	1879	1883	1892	rVB4	146695	233891	2.44%	0.535%
54	12.513	1902	1907	1913	rBV	126698	147903	1.54%	0.338%
55	12.580	1913	1918	1920	rBV	81284	102594	1.07%	0.234%
56	12.666	1927	1932	1935	rBV	104076	126176	1.31%	0.288%
57	12.757	1942	1947	1954	rBV3	93177	199344	2.08%	0.456%
58	12.897	1965	1970	1975	rVB2	67457	96528	1.01%	0.221%
59	12.970	1975	1982	1986	rVV	77174	113110	1.18%	0.259%
60	13.013	1986	1989	1995	rVB	127581	150625	1.57%	0.344%
61	13.342	2039	2043	2048	rBV2	97500	130591	1.36%	0.298%
62	14.690	2252	2264	2268	rBV	82783	124062	1.29%	0.284%
63	14.836	2283	2288	2297	rBV	90321	128654	1.34%	0.294%

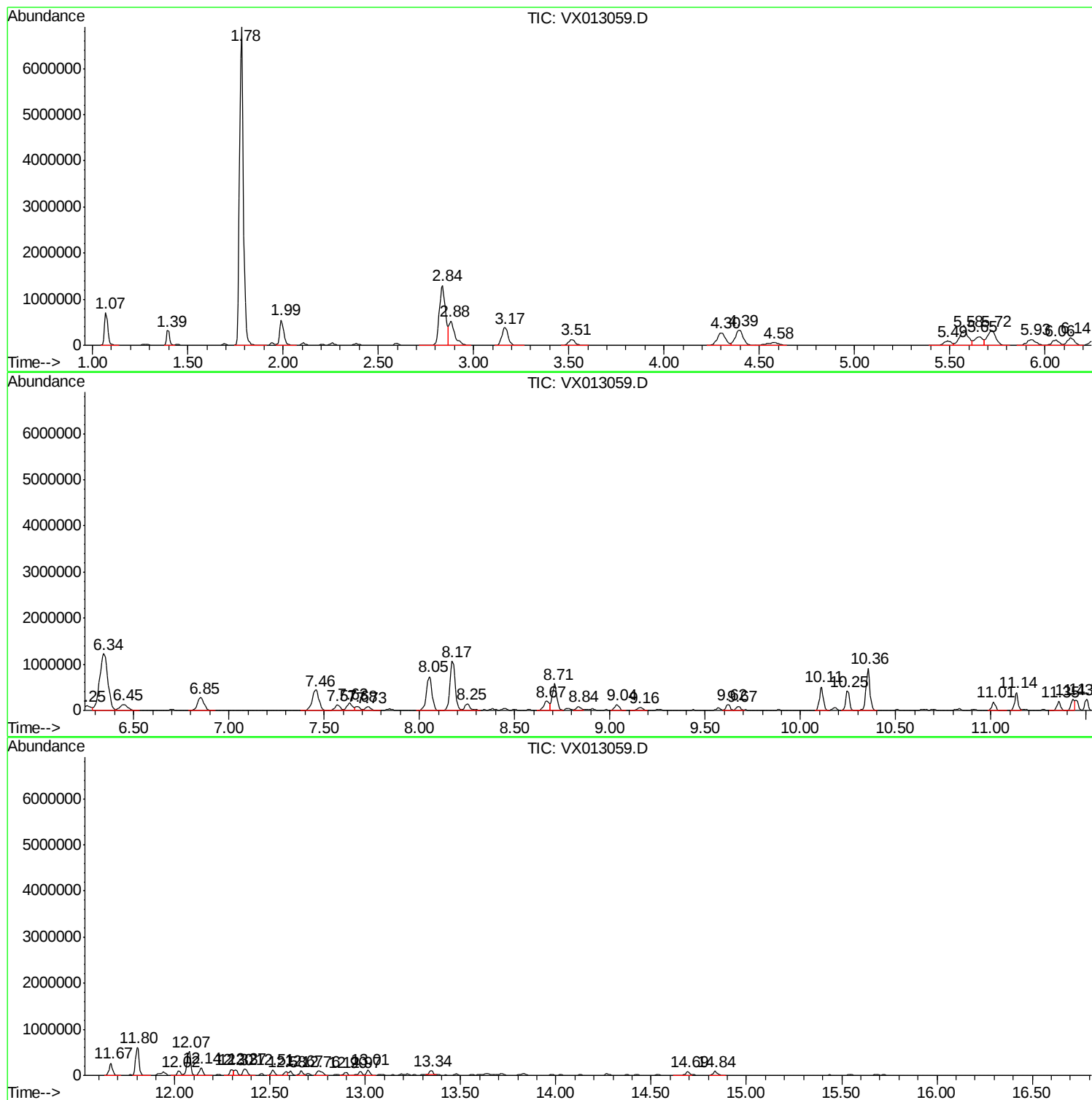
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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



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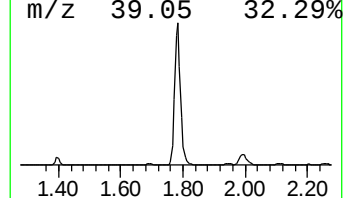
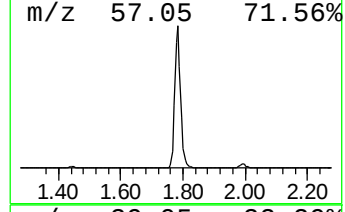
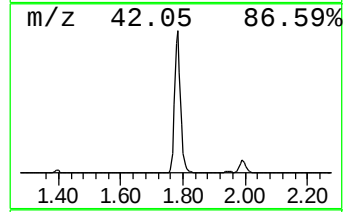
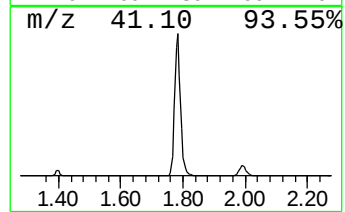
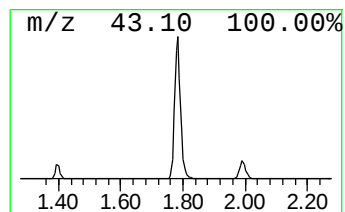
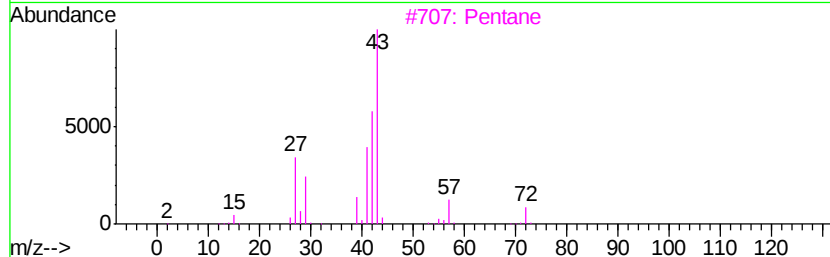
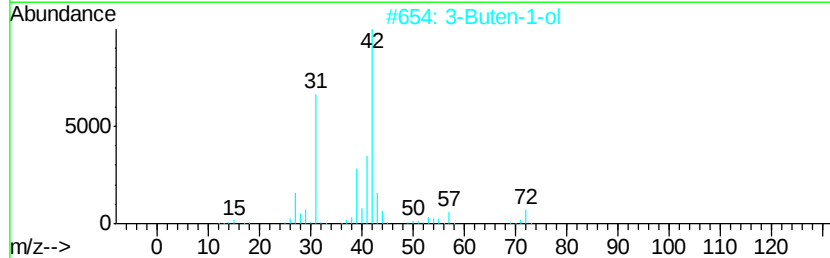
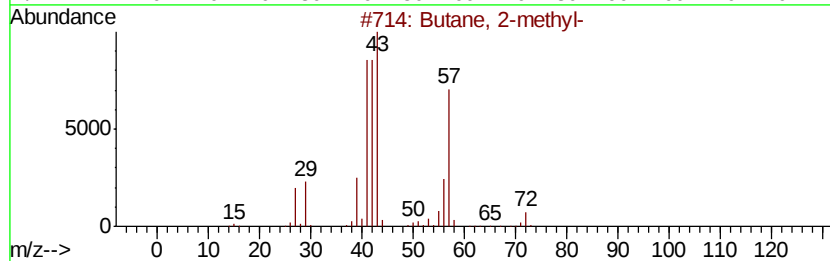
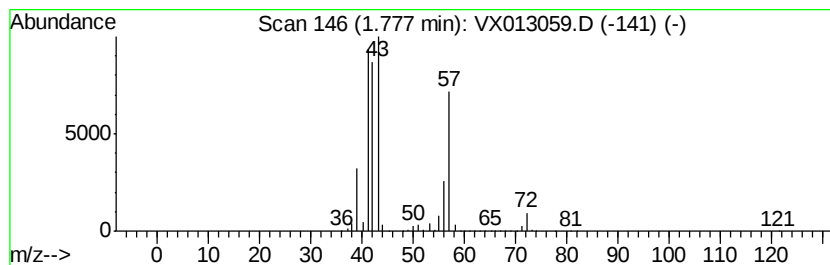
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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	890.67 ug/l	9599700	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	42
4		Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	10
5		1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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ALS Vial : 24 Sample Multiplier: 1

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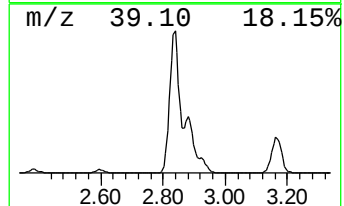
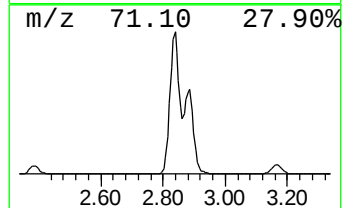
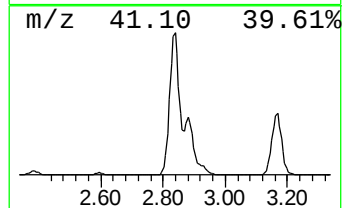
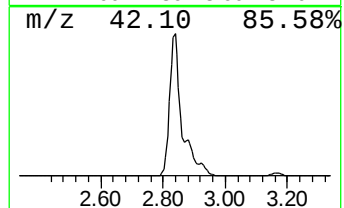
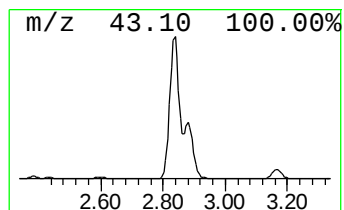
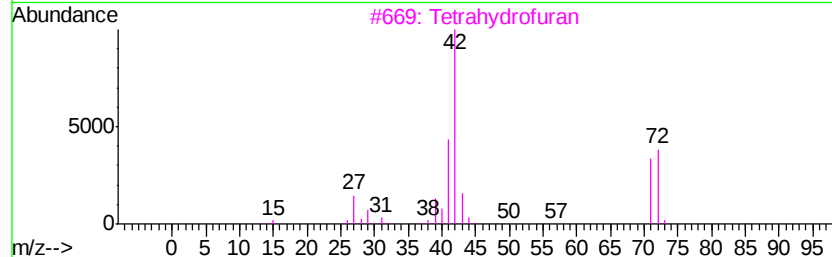
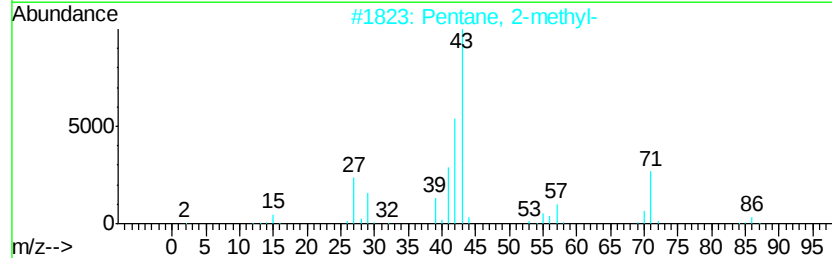
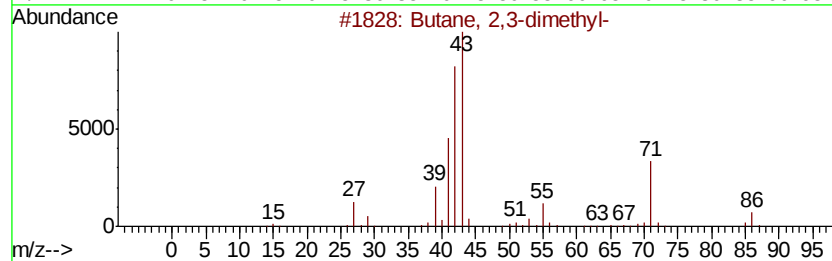
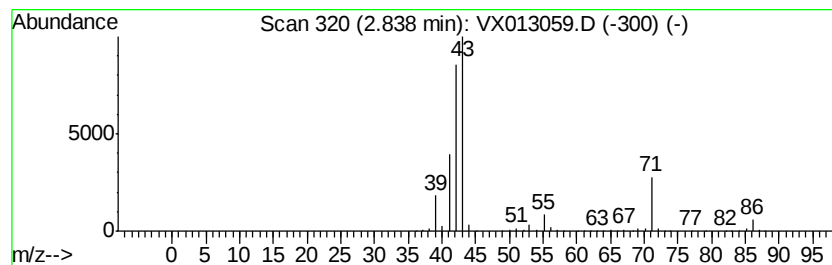
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	278.18 ug/l	2998190	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		Tetrahydrofuran	72	C4H8O	000109-99-9	38
4		Butane, 2-methyl-	72	C5H12	000078-78-4	36
5		Pyrrolidine	71	C4H9N	000123-75-1	22



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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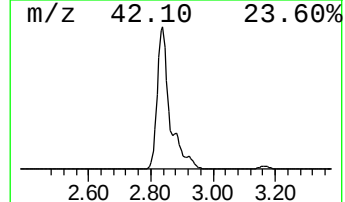
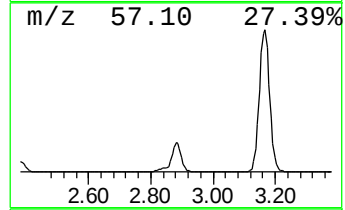
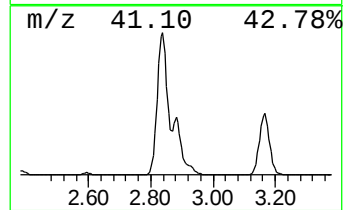
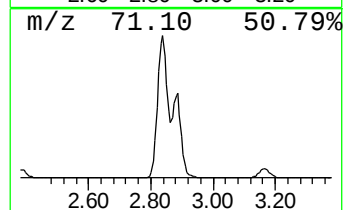
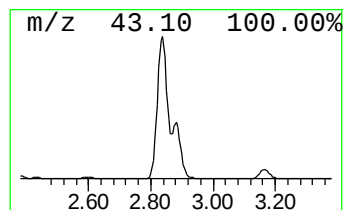
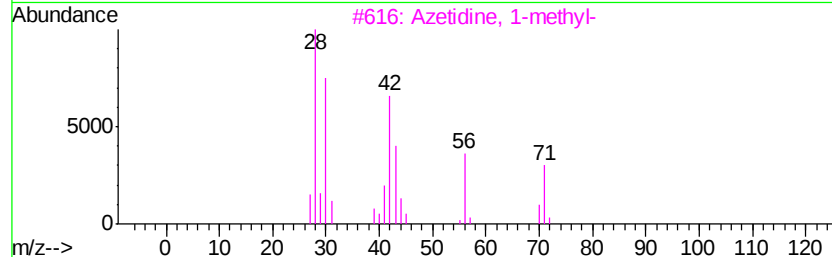
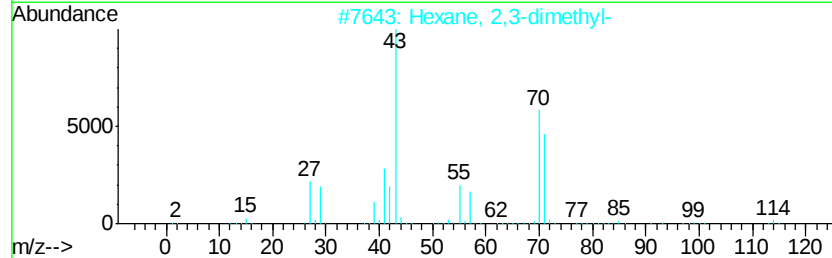
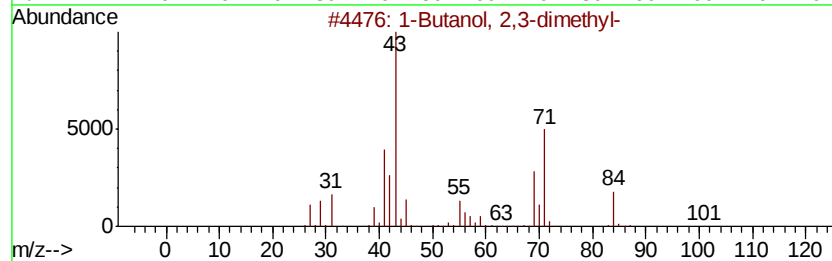
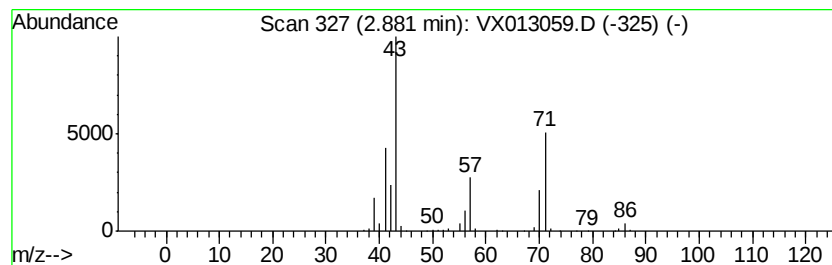
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Quant Title : SW846 8260

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

Peak Number 4 unknown2.88 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.88	96.01 ug/l	1034820	Pentafluorobenzene	5.65

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	38
2			Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	36
3			Azetidine, 1-methyl-	71	C4H9N	004923-79-9	36
4			Azetidine, 2-methyl-	71	C4H9N	019812-49-8	36
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	33



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ALS Vial : 24 Sample Multiplier: 1

Instrument :
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ClientSampled :
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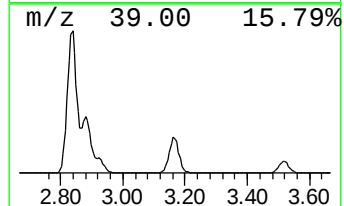
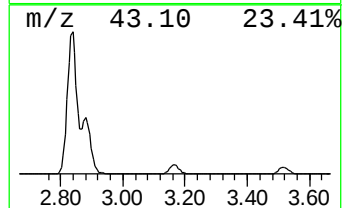
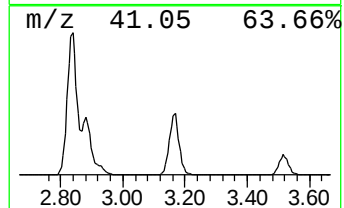
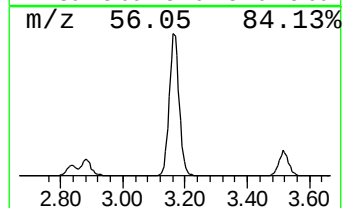
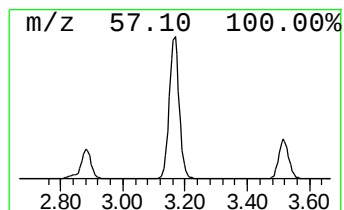
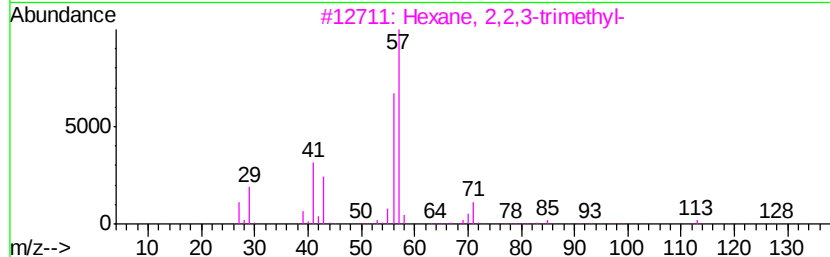
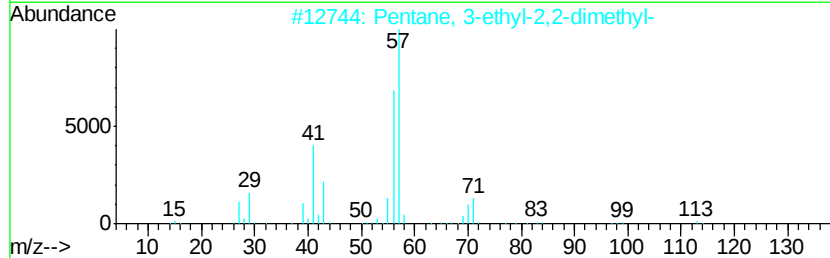
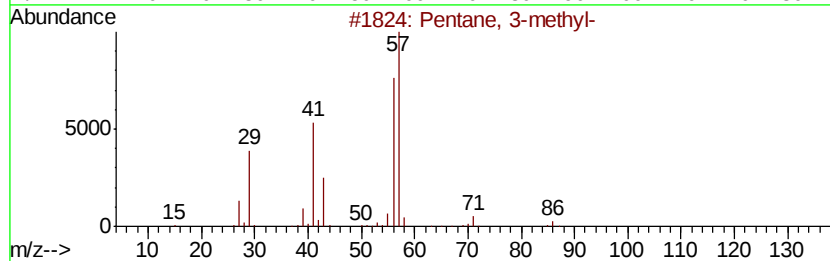
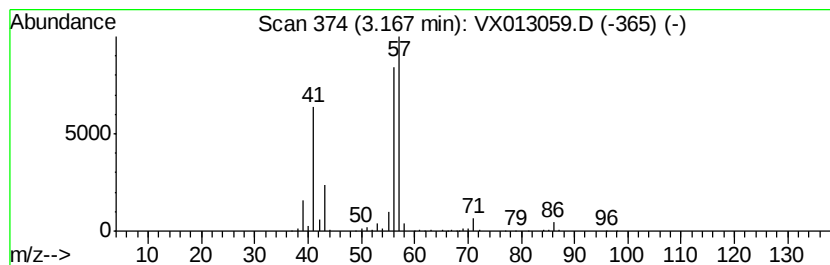
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	80.87 ug/l	871649	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2		Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
3		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	43
4		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	42
5		Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40



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FA19-JBW7333

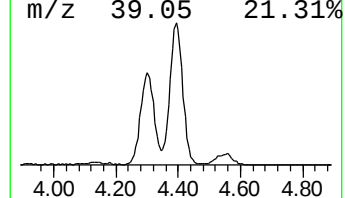
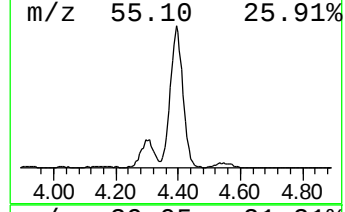
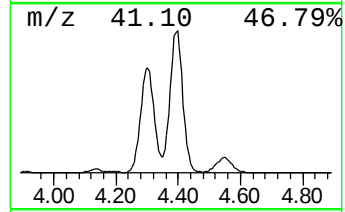
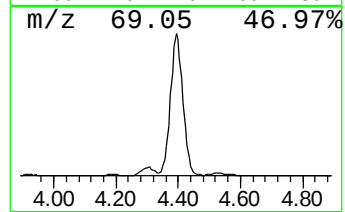
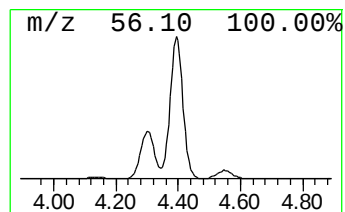
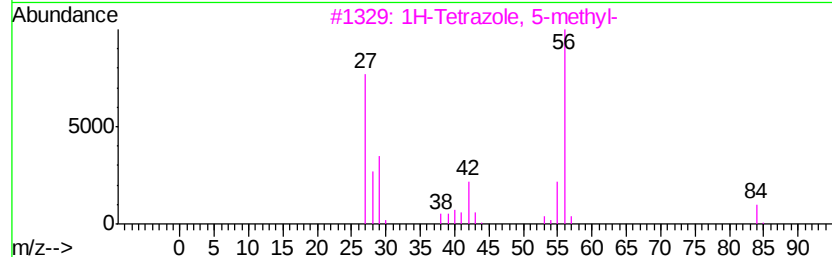
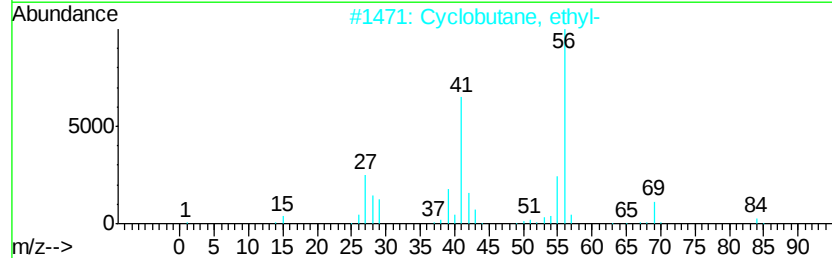
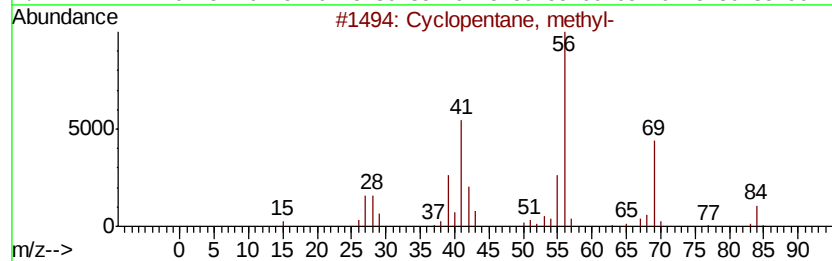
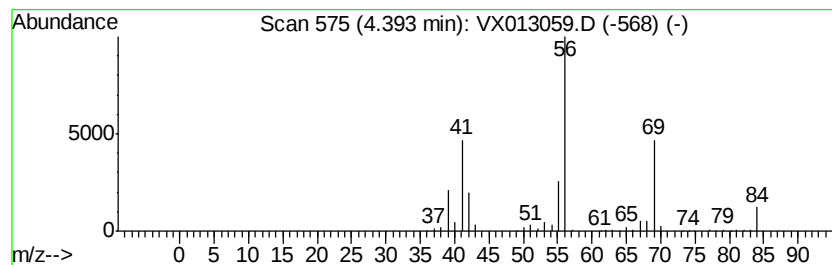
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Quant Title : SW846 8260

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

Peak Number 6 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.39	87.12 ug/l	939001	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	72
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43
5		Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	40



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013059.D
Acq On : 14 Oct 2019 18:03
Operator : JC/SP
Sample : K5313-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333

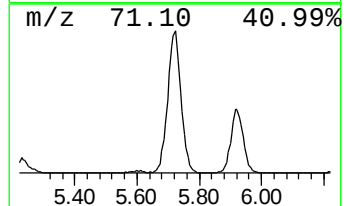
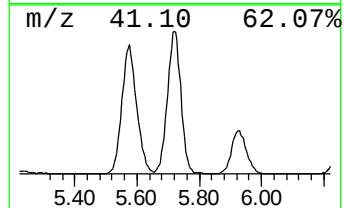
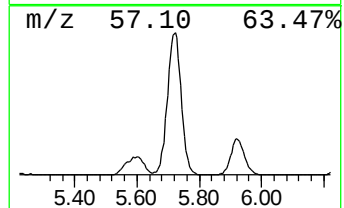
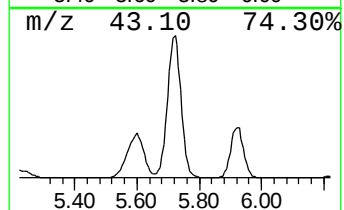
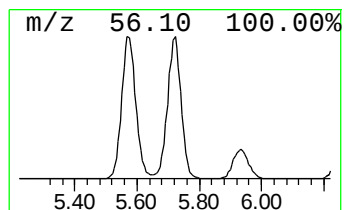
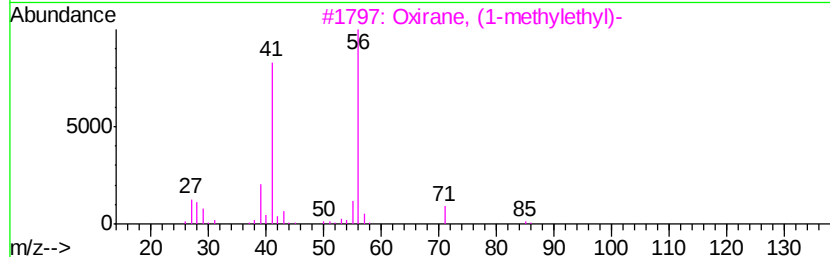
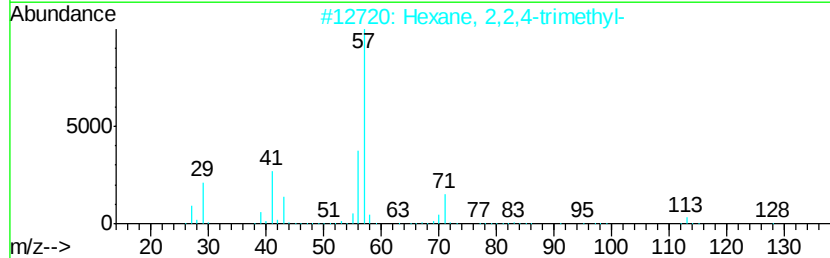
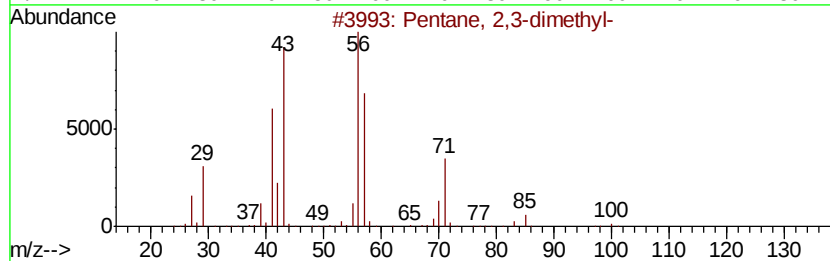
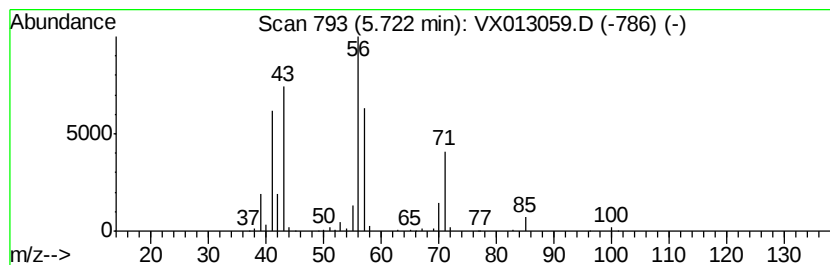
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Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.72	90.73 ug/l	977841	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		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	38
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	38
5		Heptane	100	C7H16	000142-82-5	38



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013059.D
Acq On : 14 Oct 2019 18:03
Operator : JC/SP
Sample : K5313-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333

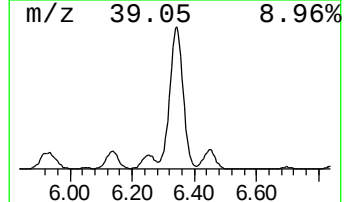
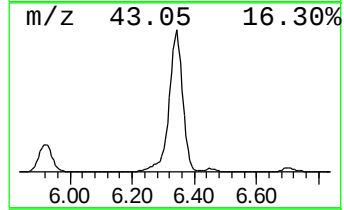
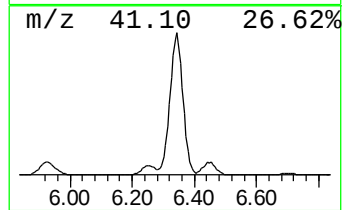
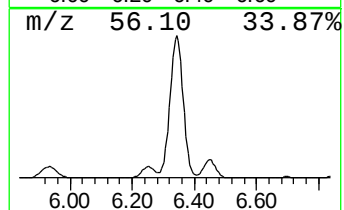
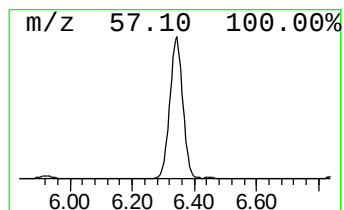
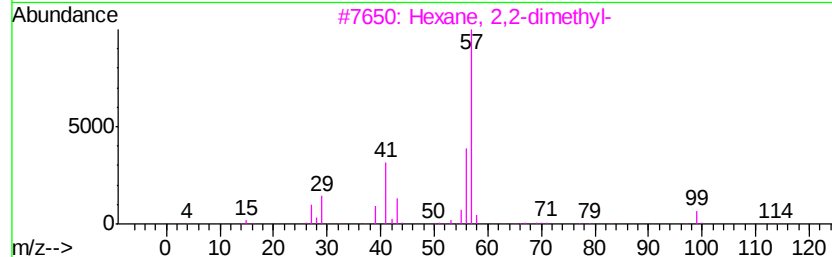
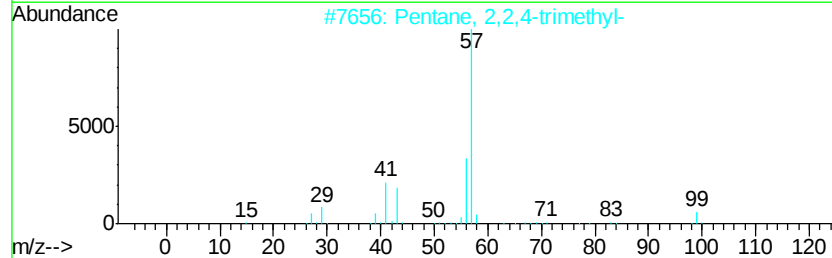
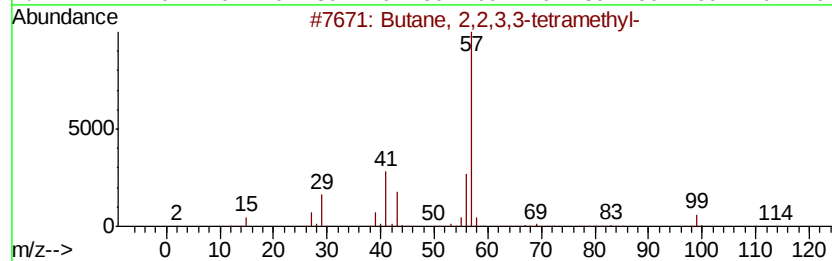
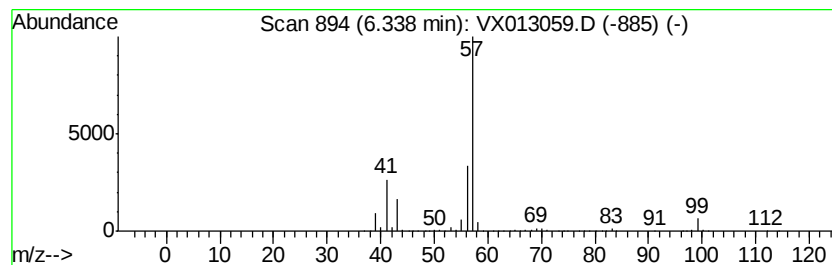
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Quant Title : SW846 8260

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

Peak Number 8 Butane, 2,2,3,3-tetramethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	281.50 ug/l	3673470	1,4-Difluorobenzene	6.85

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		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	72
4		Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	64
5		Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013059.D
Acq On : 14 Oct 2019 18:03
Operator : JC/SP
Sample : K5313-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333

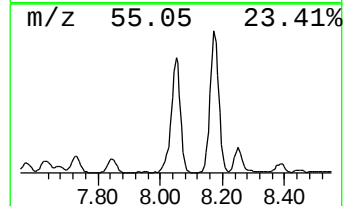
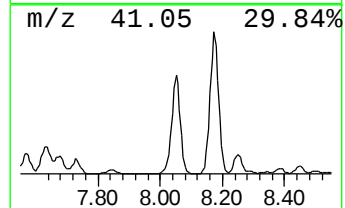
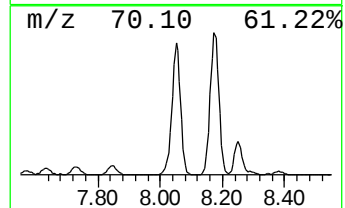
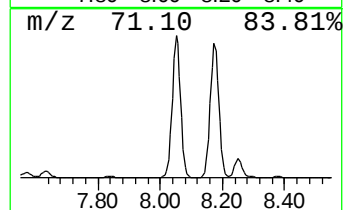
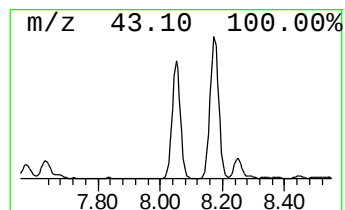
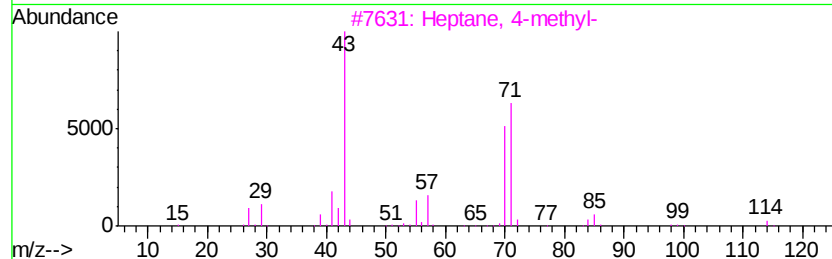
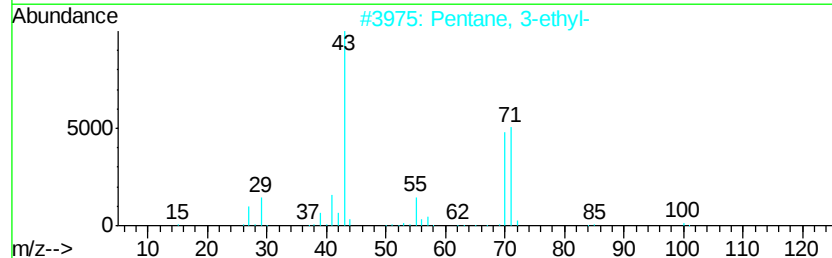
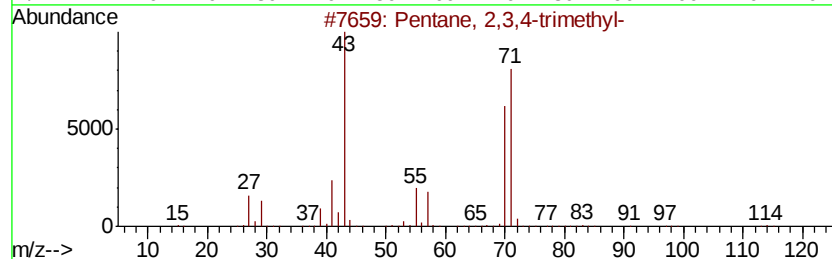
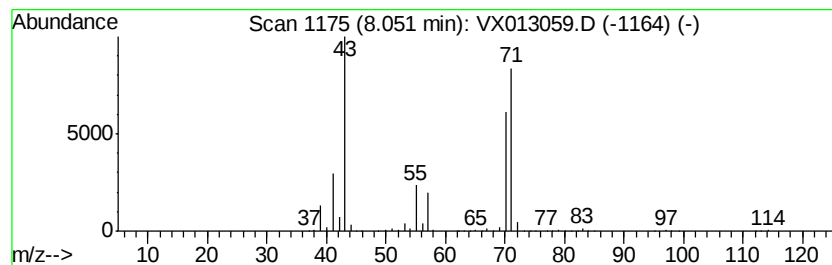
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 9 Pentane, 2,3,4-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.05	113.40 ug/l	1479830	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		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Hexane, 3,3,4-trimethyl-	128	C9H20	016747-31-2	78



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013059.D
Acq On : 14 Oct 2019 18:03
Operator : JC/SP
Sample : K5313-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333

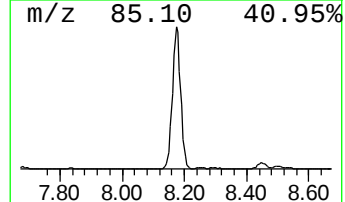
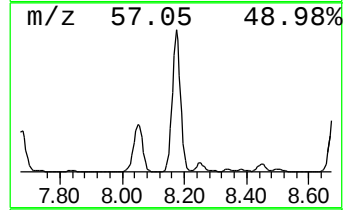
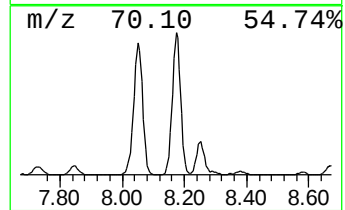
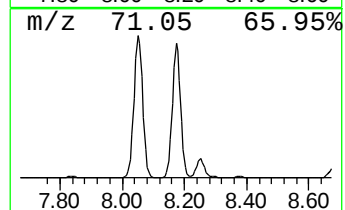
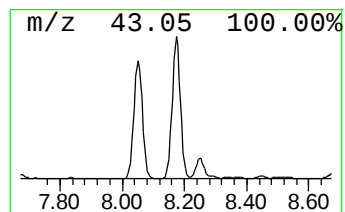
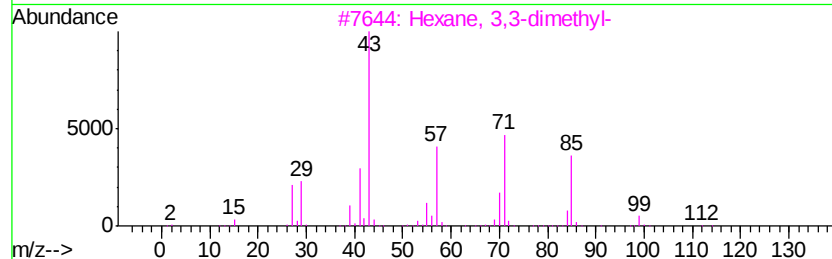
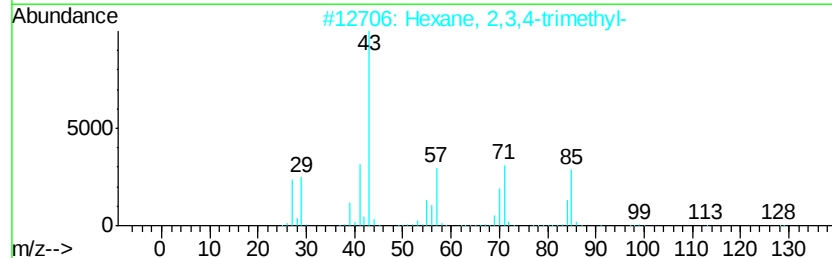
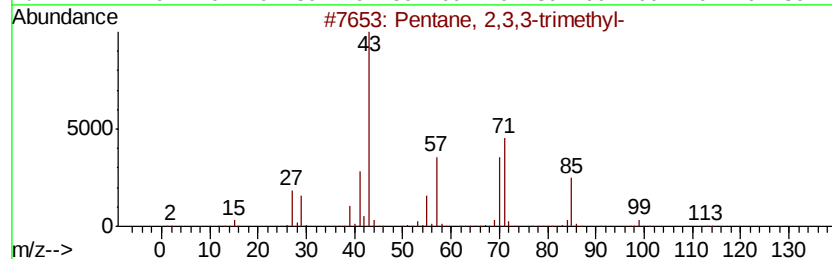
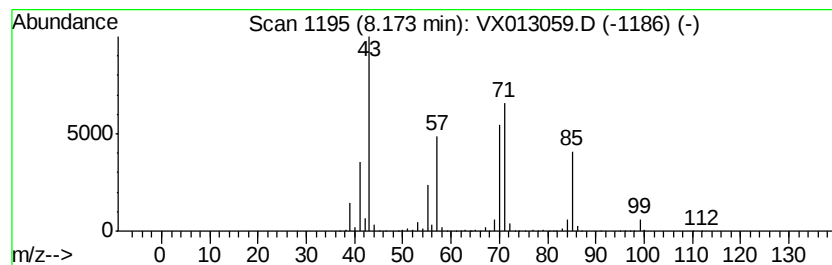
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.17	157.90 ug/l	2060550	1,4-Difluorobenzene	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	90
2		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	50



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX101419\
Data File : VX013059.D
Acq On : 14 Oct 2019 18:03
Operator : JC/SP
Sample : K5313-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333

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	890.7	ug/l	9599700	1	5.65	538903	50.0
Butane, 2,3-dimet...	2.84	278.2	ug/l	2998190	1	5.65	538903	50.0
unknown2.88	2.88	96.0	ug/l	1034820	1	5.65	538903	50.0
Pentane, 3-methyl-	3.17	80.9	ug/l	871649	1	5.65	538903	50.0
Cyclopentane, met...	4.39	87.1	ug/l	939001	1	5.65	538903	50.0
Pentane, 2,3-dime...	5.72	90.7	ug/l	977841	1	5.65	538903	50.0
Butane, 2,2,3,3-t...	6.34	281.5	ug/l	3673470	2	6.85	652477	50.0
Pentane, 2,3,4-tr...	8.05	113.4	ug/l	1479830	2	6.85	652477	50.0
Pentane, 2,3,3-tr...	8.17	157.9	ug/l	2060550	2	6.85	652477	50.0