

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX101419\
 Data File : VX013060.D
 Acq On : 14 Oct 2019 18:26
 Operator : JC/SP
 Sample : K5313-05
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FA19-JBW7333-9001

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	42	rBV	682091	844555	8.98%	1.917%
2	1.399	80	84	89	rBV	305511	322136	3.43%	0.731%
3	1.783	141	147	162	rBV	6846180	9401618	100.00%	21.339%
4	1.990	177	181	195	rVB2	549904	851072	9.05%	1.932%
5	2.594	270	280	296	rBV	54711	105004	1.12%	0.238%
6	2.838	310	320	325	rBV	1280786	2935577	31.22%	6.663%
7	2.880	325	327	344	rVB	538211	1053085	11.20%	2.390%
8	3.167	362	374	390	rBV	376263	872803	9.28%	1.981%
9	3.514	420	431	445	rBV	133209	305339	3.25%	0.693%
10	4.301	547	560	568	rBV	279870	846854	9.01%	1.922%
11	4.392	568	575	589	rVB	320438	933565	9.93%	2.119%
12	4.581	589	606	617	rBV5	58505	253089	2.69%	0.574%
13	5.490	740	755	761	rBV2	95713	284320	3.02%	0.645%
14	5.575	761	769	776	rVV3	314734	1050161	11.17%	2.384%
15	5.654	776	782	786	rVV	191799	545204	5.80%	1.237%
16	5.721	786	793	811	rVV	318964	993553	10.57%	2.255%
17	5.929	814	827	839	rVV4	127046	433062	4.61%	0.983%
18	6.057	839	848	854	rVV	112195	293765	3.12%	0.667%
19	6.136	854	861	871	rVV	167360	441742	4.70%	1.003%
20	6.252	871	880	885	rVV2	99827	285091	3.03%	0.647%
21	6.343	885	895	906	rVV	1222668	3689872	39.25%	8.375%
22	6.447	906	912	925	rVB2	123998	334429	3.56%	0.759%
23	6.849	969	978	989	rBV	275693	656132	6.98%	1.489%
24	7.459	1064	1078	1087	rBV	449232	1068943	11.37%	2.426%
25	7.568	1088	1096	1101	rVV	118063	244988	2.61%	0.556%
26	7.636	1101	1107	1111	rVV	159022	359951	3.83%	0.817%
27	7.672	1111	1113	1118	rVV	85587	154607	1.64%	0.351%
28	7.727	1118	1122	1134	rVV	78024	152457	1.62%	0.346%
29	8.050	1164	1175	1186	rBV	759592	1499342	15.95%	3.403%
30	8.172	1186	1195	1203	rBV	1021196	2028982	21.58%	4.605%
31	8.251	1203	1208	1214	rVV	130432	219022	2.33%	0.497%
32	8.666	1267	1276	1279	rBV3	206385	410303	4.36%	0.931%
33	8.709	1279	1283	1290	rVB	576854	934588	9.94%	2.121%
34	8.837	1299	1304	1308	rBV	70357	114064	1.21%	0.259%

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35	9.038	1331	1337	1343	rVB	127026	203649	2.17%	0.462%
36	9.160	1348	1357	1363	rBV	69212	118905	1.26%	0.270%
37	9.617	1428	1432	1437	rVV	124753	175110	1.86%	0.397%
38	9.672	1437	1441	1446	rVV	80575	119443	1.27%	0.271%
39	10.111	1507	1513	1519	rBV	535631	714254	7.60%	1.621%
40	10.245	1530	1535	1544	rVB	408015	556147	5.92%	1.262%
41	10.355	1544	1553	1560	rBV	918999	1249445	13.29%	2.836%
42	11.013	1656	1661	1675	rVB	195366	246719	2.62%	0.560%
43	11.135	1675	1681	1686	rBV	390557	522360	5.56%	1.186%
44	11.354	1710	1717	1724	rBV	190623	248817	2.65%	0.565%
45	11.428	1724	1729	1731	rVV	235374	313452	3.33%	0.711%
46	11.452	1731	1733	1737	rVV	220620	234232	2.49%	0.532%
47	11.501	1737	1741	1750	rVB	256881	302260	3.21%	0.686%
48	11.665	1762	1768	1777	rBV	266193	346448	3.68%	0.786%
49	11.806	1786	1791	1801	rVB	625792	776771	8.26%	1.763%
50	11.940	1811	1813	1819	rVB	81477	95062	1.01%	0.216%
51	12.019	1819	1826	1830	rBV	97997	126344	1.34%	0.287%
52	12.074	1830	1835	1841	rVV2	523450	702178	7.47%	1.594%
53	12.141	1841	1846	1851	rVB	169534	216214	2.30%	0.491%
54	12.299	1865	1872	1873	rBV2	126534	157800	1.68%	0.358%
55	12.318	1873	1875	1879	rVV	135718	157738	1.68%	0.358%
56	12.366	1879	1883	1892	rVB4	159261	243311	2.59%	0.552%
57	12.513	1903	1907	1913	rBV	122966	149441	1.59%	0.339%
58	12.580	1913	1918	1920	rBV	81108	103258	1.10%	0.234%
59	12.604	1920	1922	1927	rVB	90793	99939	1.06%	0.227%
60	12.665	1927	1932	1935	rBV	109640	127732	1.36%	0.290%
61	12.750	1942	1946	1954	rBV4	91676	201246	2.14%	0.457%
62	12.897	1965	1970	1975	rVB3	66226	97378	1.04%	0.221%
63	12.976	1975	1983	1986	rVV	78270	116183	1.24%	0.264%
64	13.013	1986	1989	1995	rVB	127488	152315	1.62%	0.346%
65	13.342	2039	2043	2048	rBV2	100590	135516	1.44%	0.308%
66	14.835	2283	2288	2297	rVB	91185	129652	1.38%	0.294%

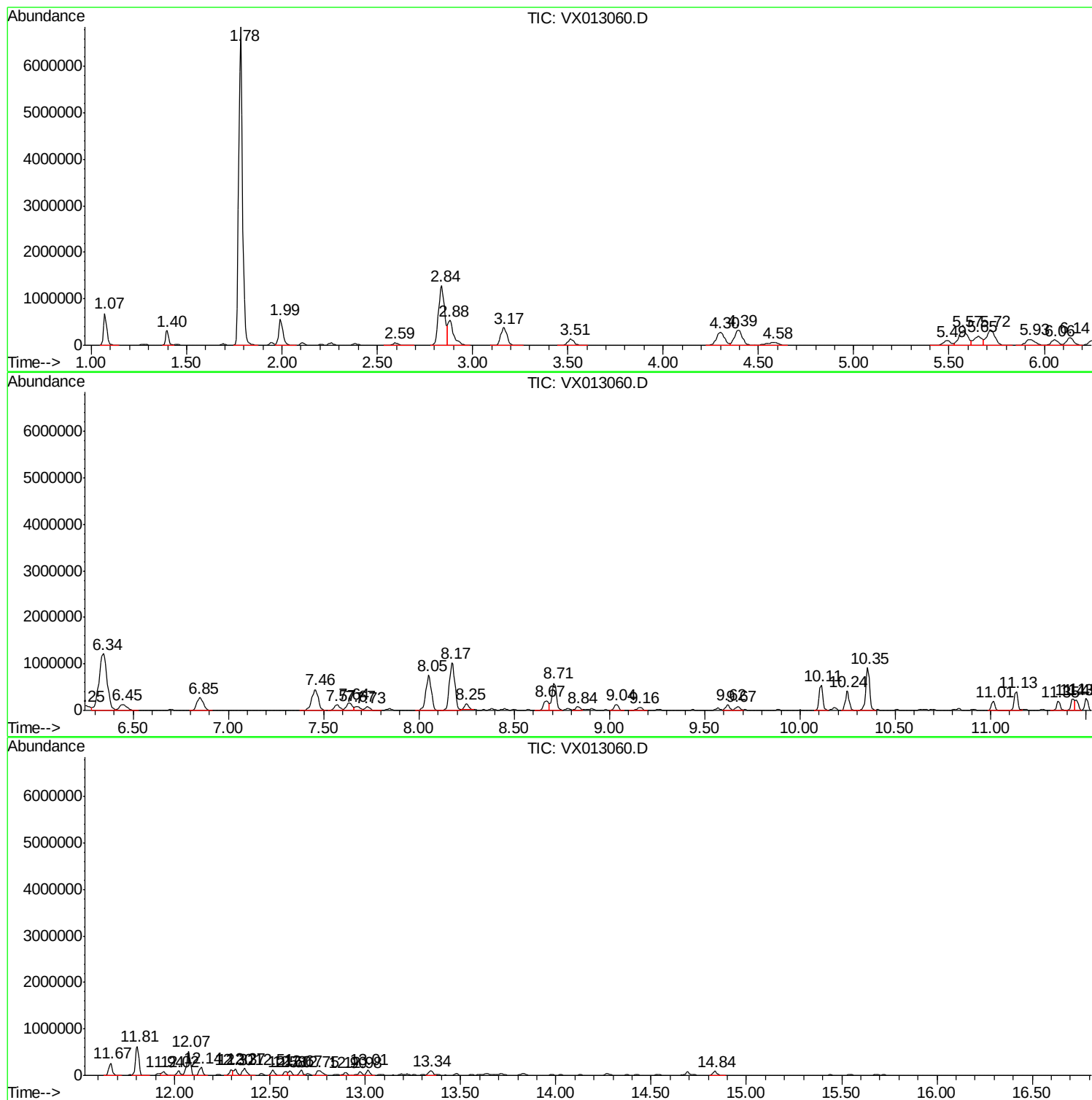
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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



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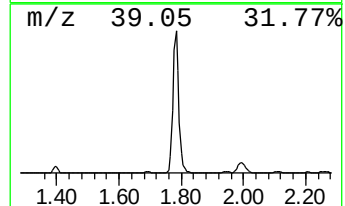
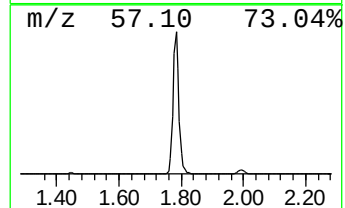
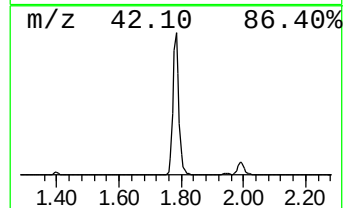
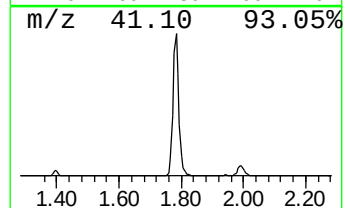
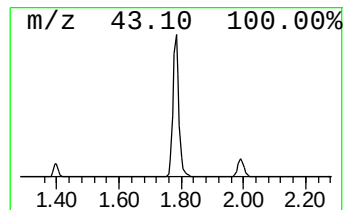
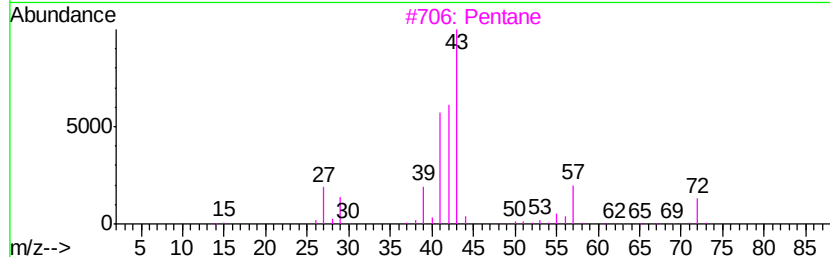
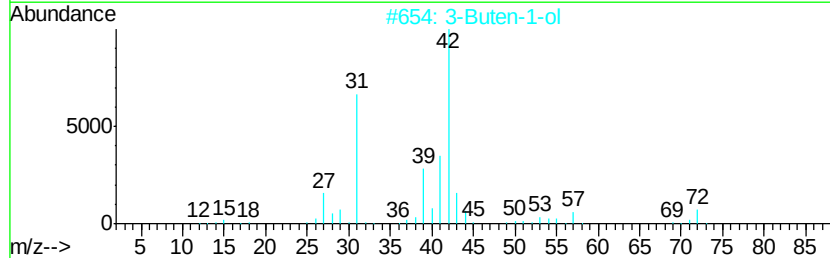
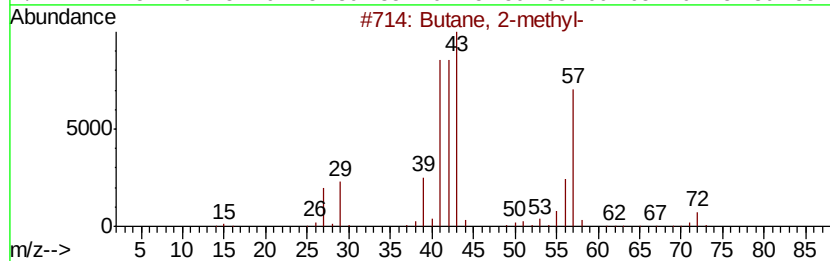
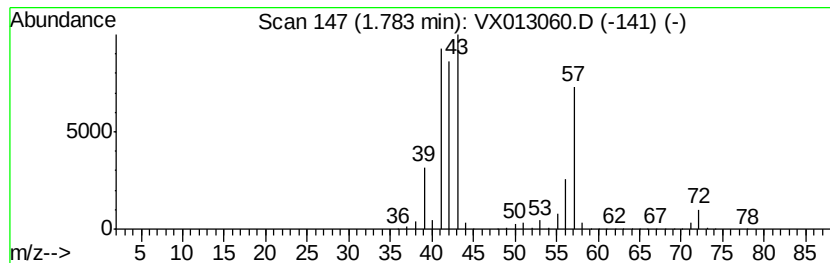
Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

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 1 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.78	862.21 ug/l	9401620	Pentafluorobenzene	5.65
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Butane, 2-methyl-	72 C5H12	000078-78-4	94
2	3-Buten-1-ol	72 C4H8O	000627-27-0	50
3	Pentane	72 C5H12	000109-66-0	36
4	1-Propene, 2-methyl-	56 C4H8	000115-11-7	14
5	1-Butene	56 C4H8	000106-98-9	10



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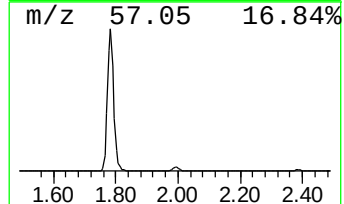
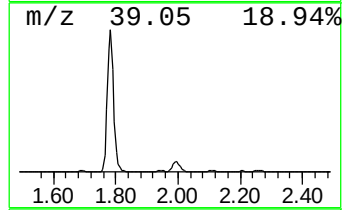
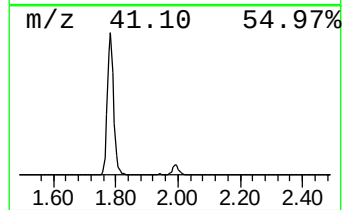
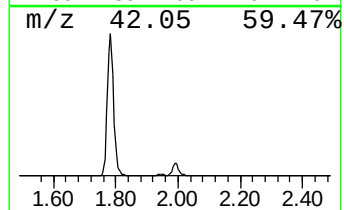
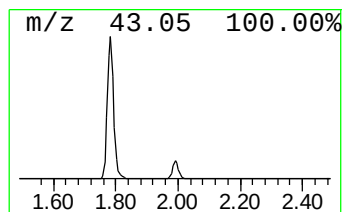
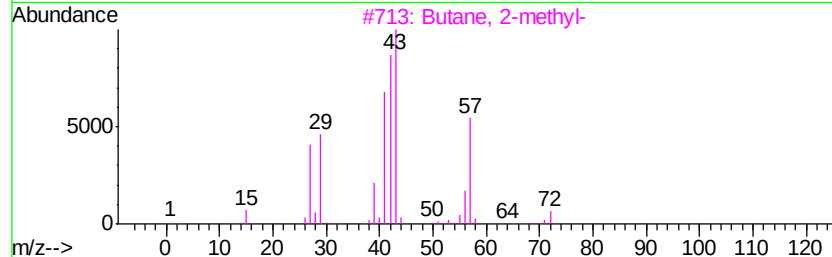
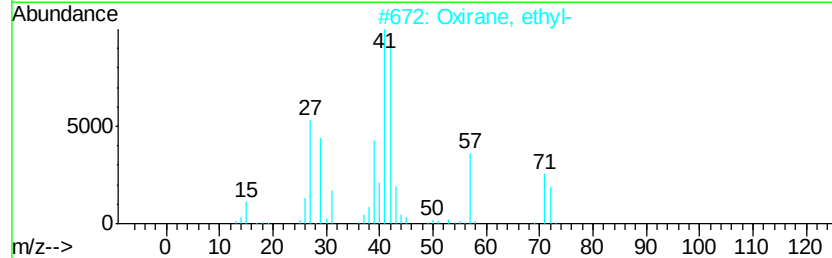
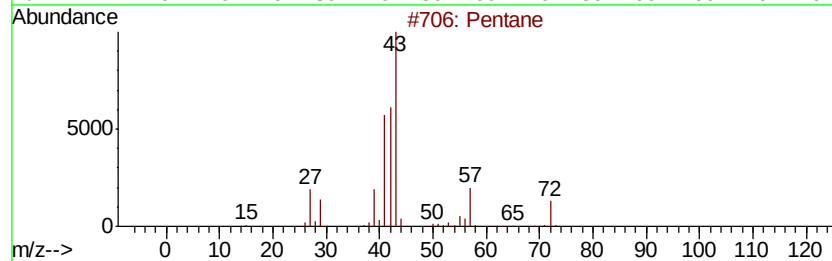
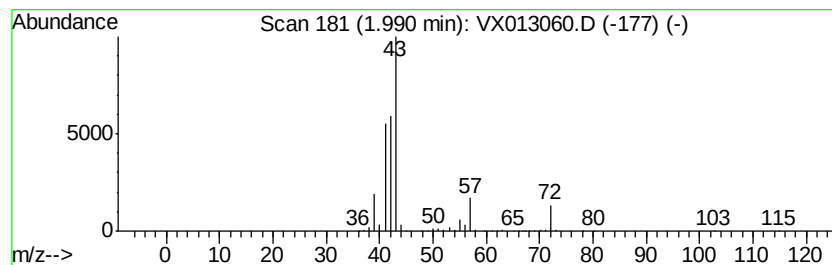
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.99	78.05 ug/l	851072	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	45
4		Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	17
5		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	9



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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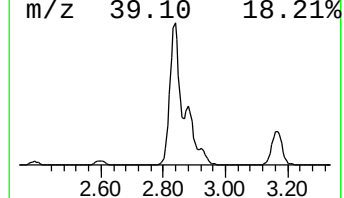
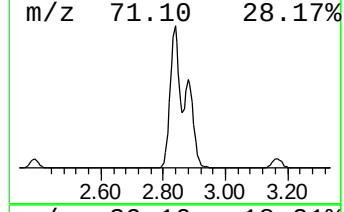
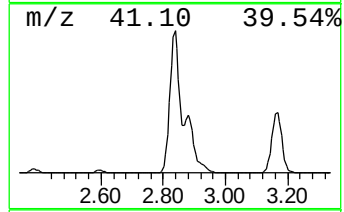
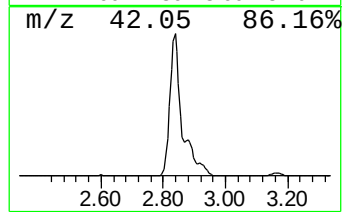
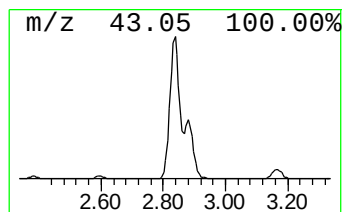
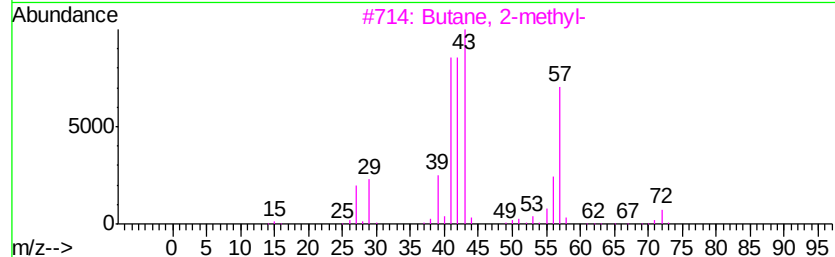
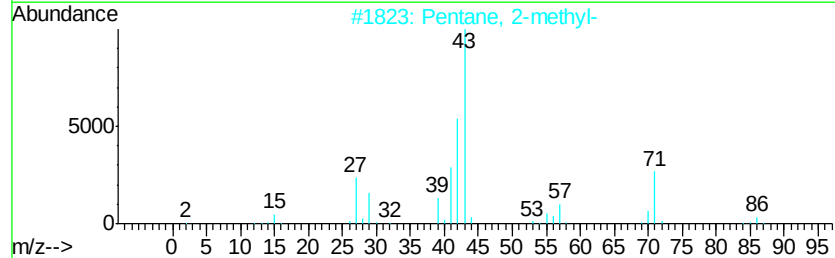
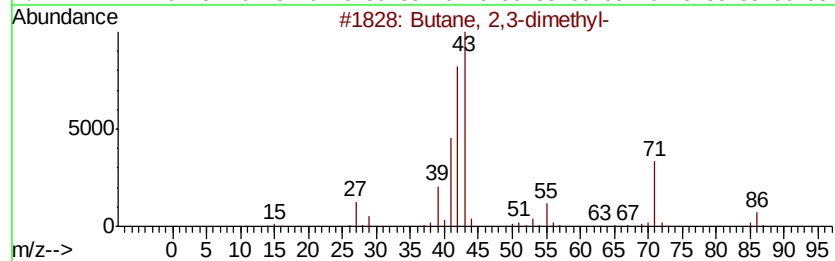
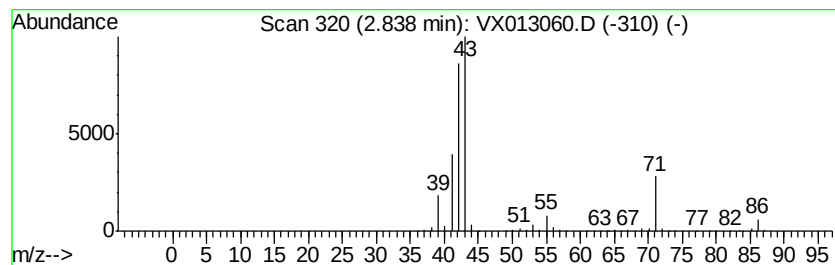
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 Butane, 2,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	269.22 ug/l	2935580	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		1-Pentene	70	C5H10	000109-67-1	28
5		Pyrrolidine	71	C4H9N	000123-75-1	22



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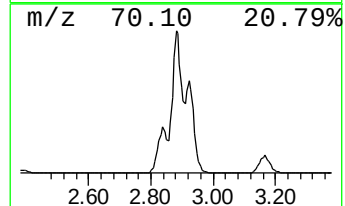
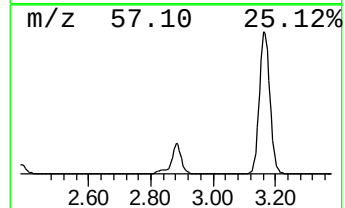
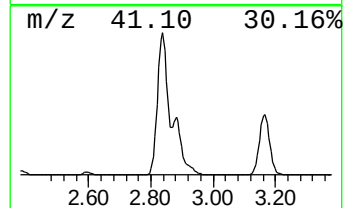
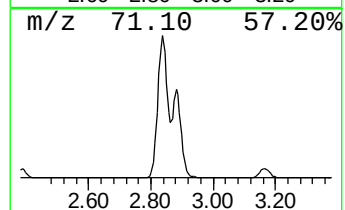
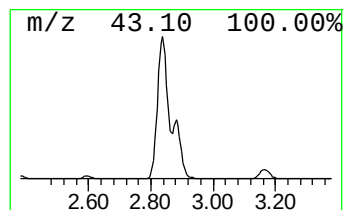
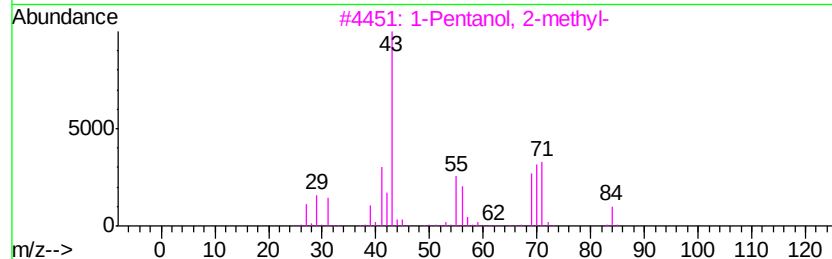
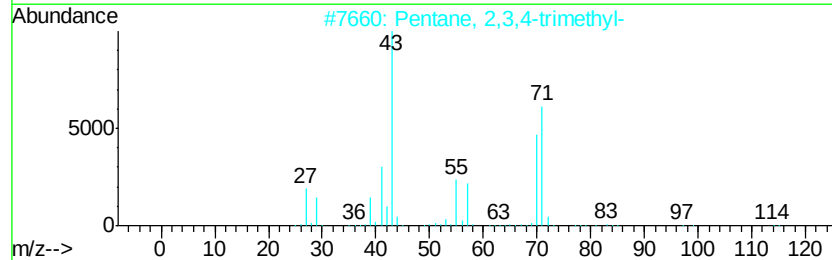
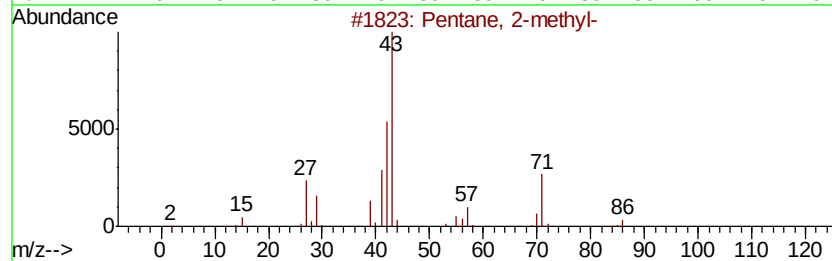
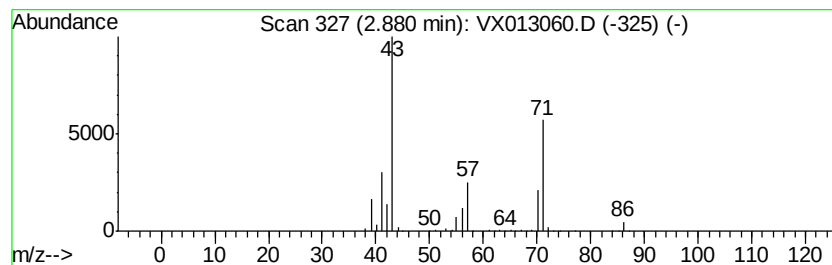
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Quant Title : SW846 8260

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	96.58 ug/l	1053090	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2-methyl-	86	C6H14	000107-83-5	38
2		Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	33
3		1-Pentanol, 2-methyl-	102	C6H14O	000105-30-6	25
4		Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	25
5		Butane, 2-methyl-	72	C5H12	000078-78-4	9



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FA19-JBW7333-9001

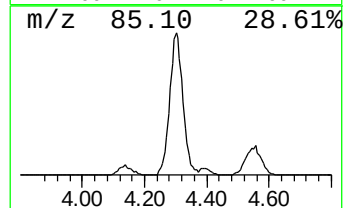
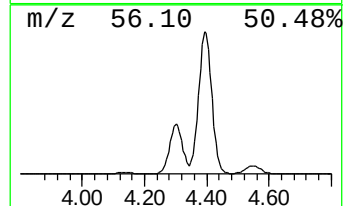
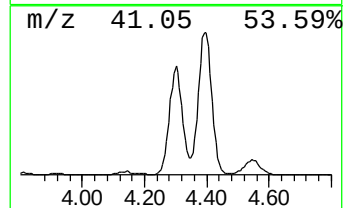
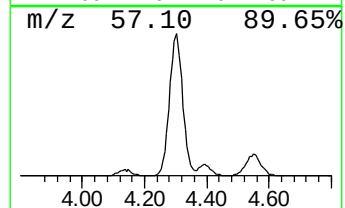
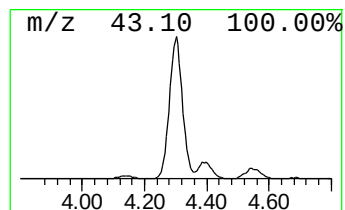
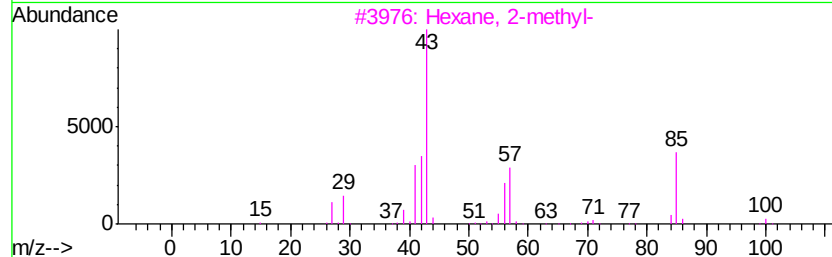
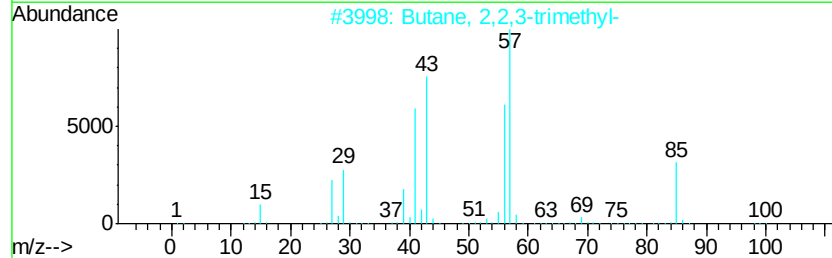
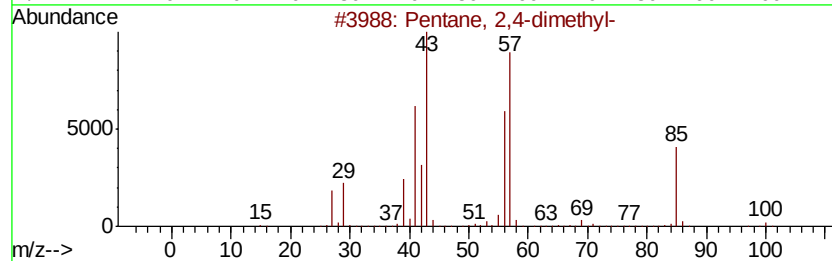
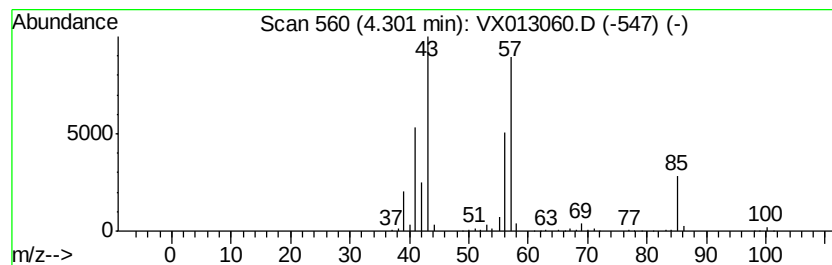
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Quant Title : SW846 8260

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

Peak Number 5 Pentane, 2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.30	77.66 ug/l	846854	Pentafluorobenzene	5.65

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 2,4-dimethyl-	100	C7H16	000108-08-7	94
2		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3		Hexane, 2-methyl-	100	C7H16	000591-76-4	64
4		Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	59
5		Oxalic acid, butyl isohexyl ester	230	C12H22O4	1000309-32-7	59



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

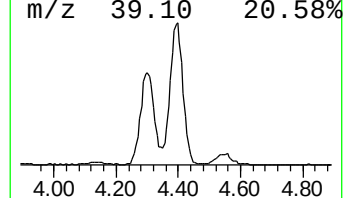
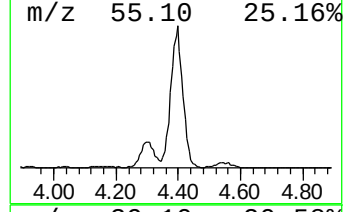
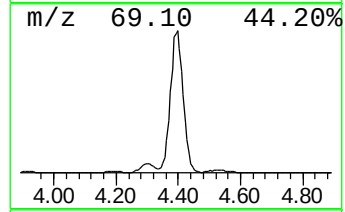
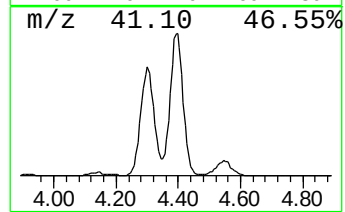
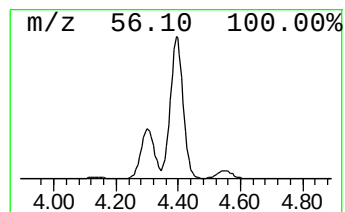
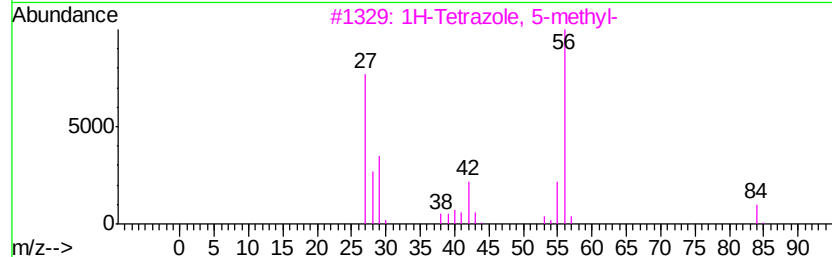
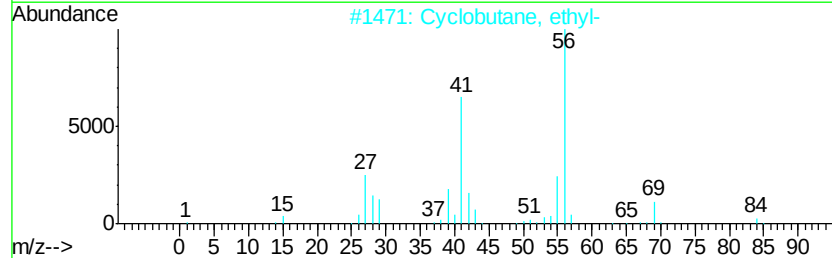
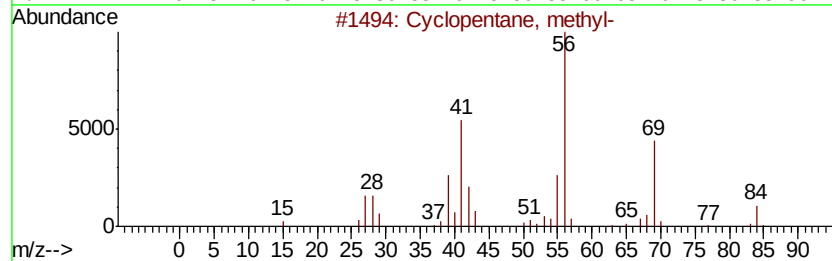
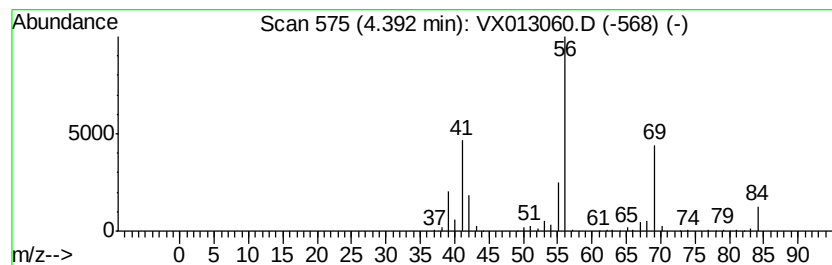
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Quant Title : SW846 8260

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	85.62 ug/l	933565	Pentafluorobenzene	5.65

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		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	64
5		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

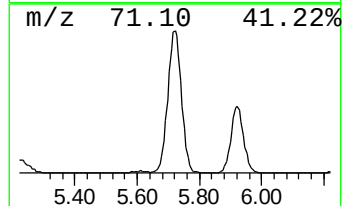
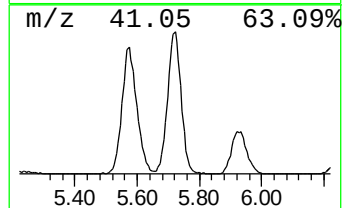
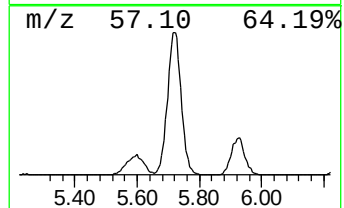
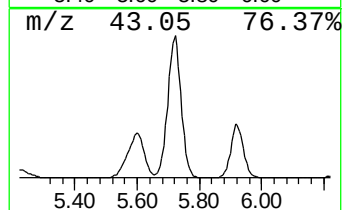
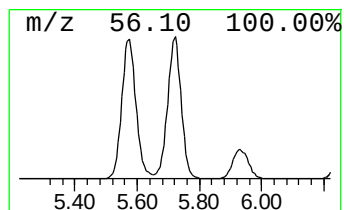
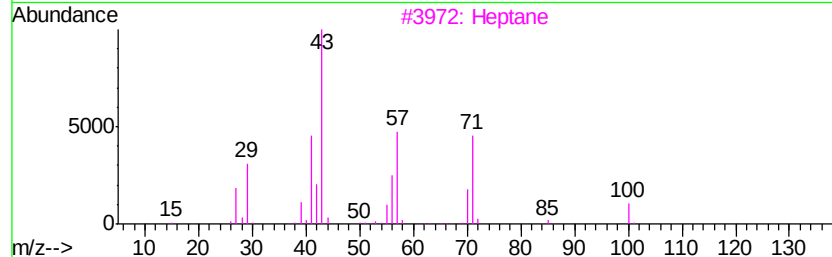
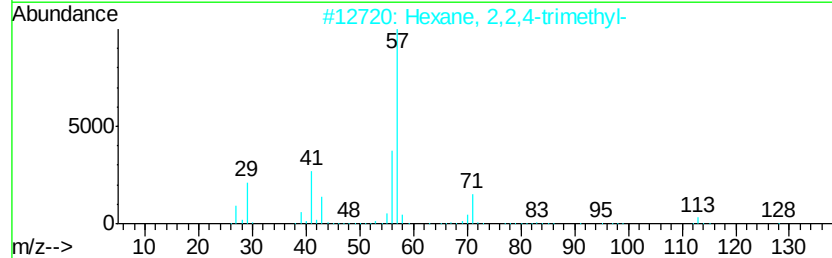
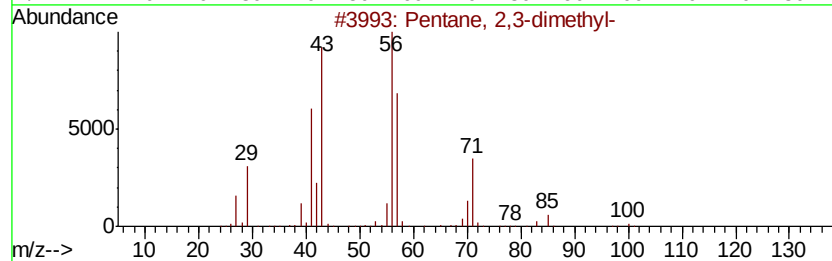
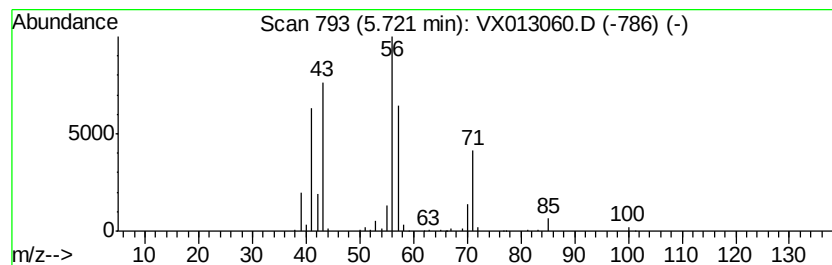
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Quant Title : SW846 8260

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	91.12 ug/l	993553	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	38
3		Heptane	100	C7H16	000142-82-5	38
4		Aziridine, 2-methyl-	57	C3H7N	000075-55-8	37
5		Propane, 1-isocyanato-	85	C4H7NO	000110-78-1	37



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

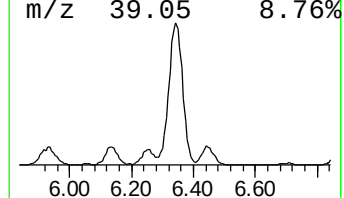
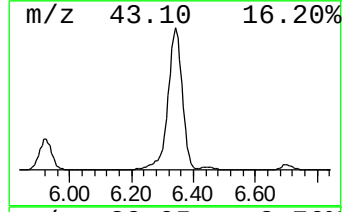
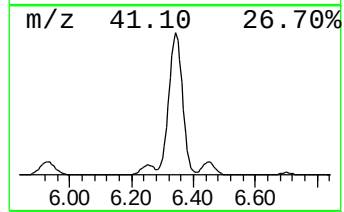
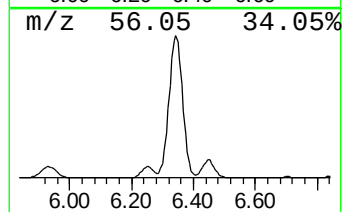
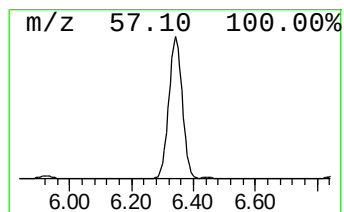
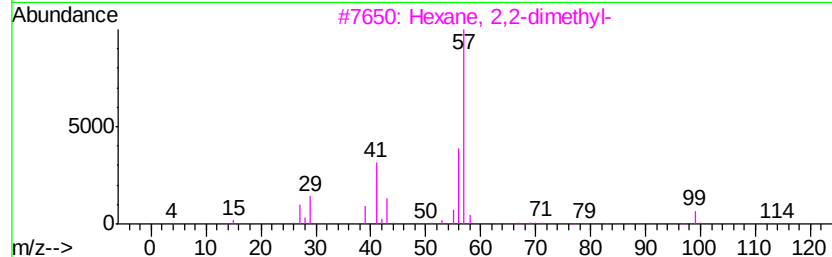
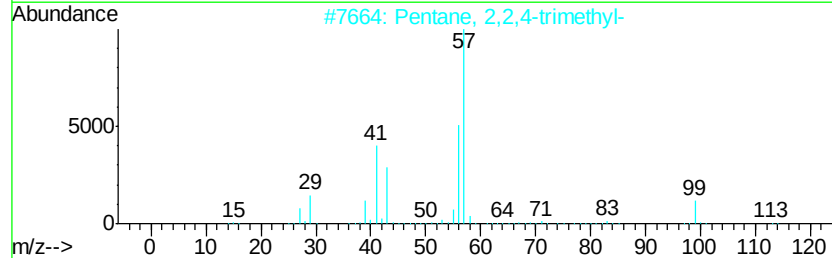
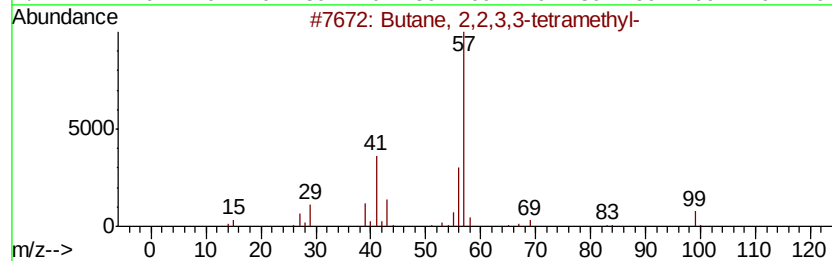
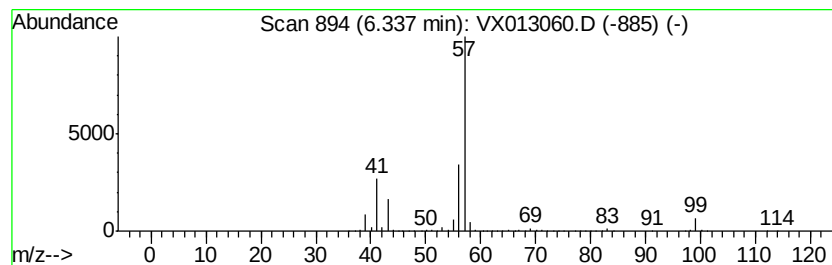
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Quant Title : SW846 8260

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	281.18 ug/l	3689870	1,4-Difluorobenzene	6.85

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	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 : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

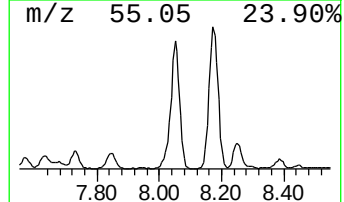
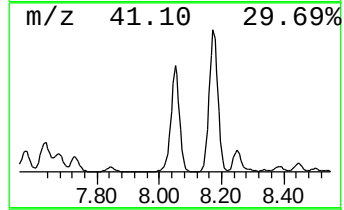
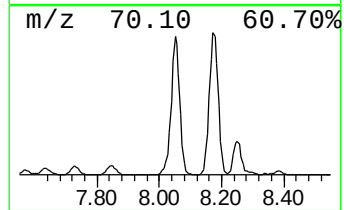
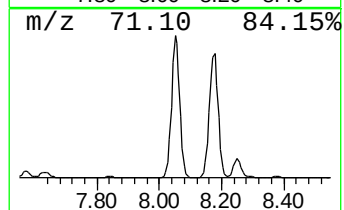
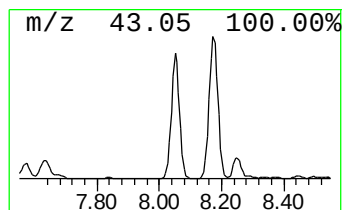
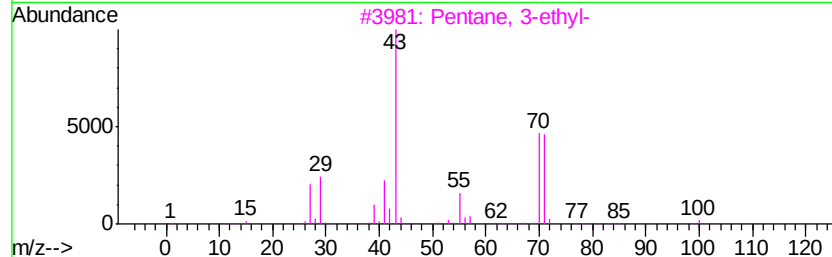
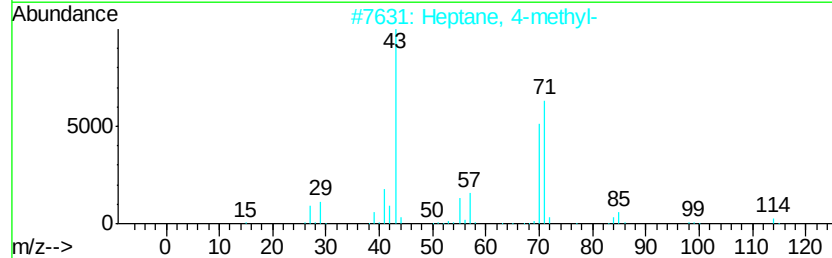
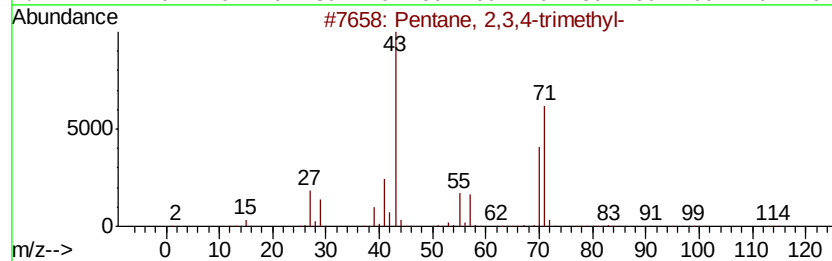
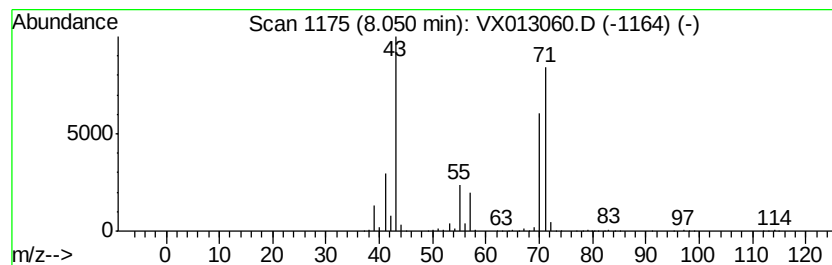
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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	114.26 ug/l	1499340	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		Heptane, 4-methyl-	114	C8H18	000589-53-7	83
3		Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	78
5		Decane, 3,3,4-trimethyl-	184	C13H28	049622-18-6	74



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA X\DATA\VX101419\
Data File : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

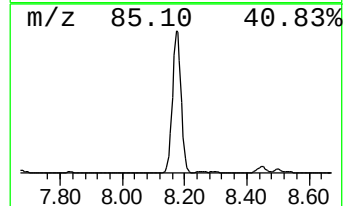
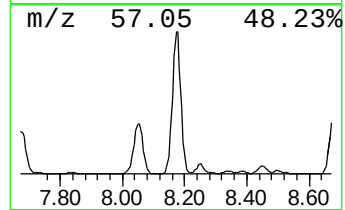
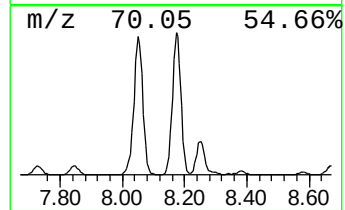
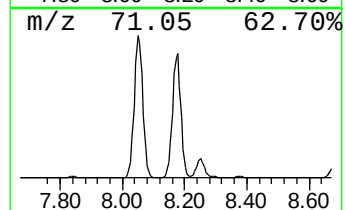
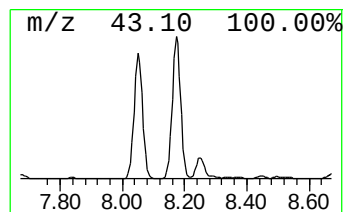
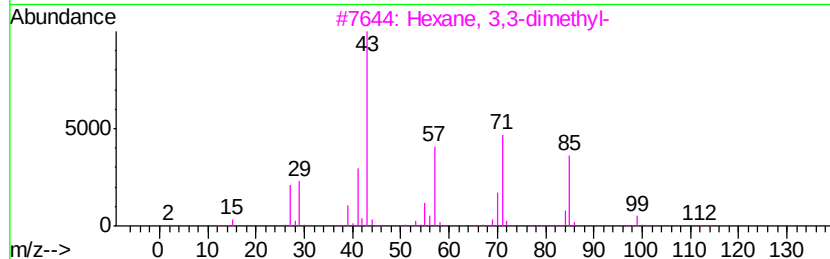
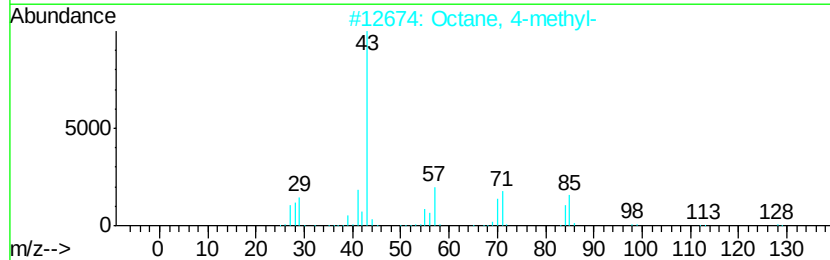
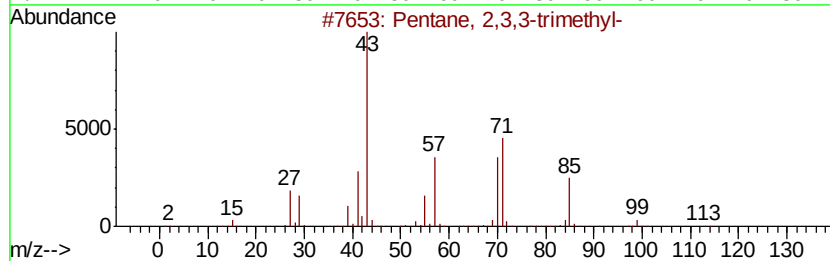
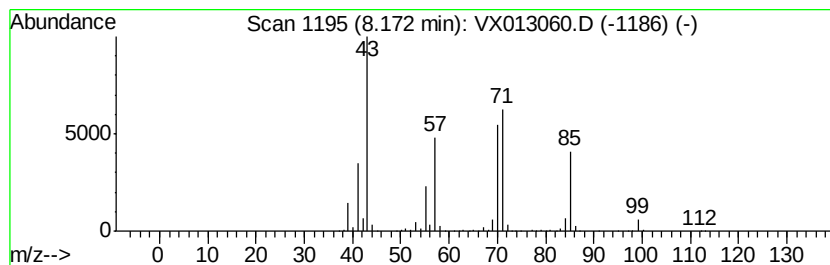
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X100819W.M
Quant Title : SW846 8260

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	154.62 ug/l	2028980	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		Octane, 4-methyl-	128	C9H20	002216-34-4	64
3		Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	64
4		Hexane, 3-methyl-	100	C7H16	000589-34-4	53
5		Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX101419\
Data File : VX013060.D
Acq On : 14 Oct 2019 18:26
Operator : JC/SP
Sample : K5313-05
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
FA19-JBW7333-9001

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Pentane	1.99	78.0	ug/l	851072	1	5.65	545204	50.0
Butane, 2,3-dimet...	2.84	269.2	ug/l	2935580	1	5.65	545204	50.0
unknown2.88	2.88	96.6	ug/l	1053090	1	5.65	545204	50.0
Pentane, 2,4-dime...	4.30	77.7	ug/l	846854	1	5.65	545204	50.0
Cyclopentane, met...	4.39	85.6	ug/l	933565	1	5.65	545204	50.0
Pentane, 2,3-dime...	5.72	91.1	ug/l	993553	1	5.65	545204	50.0
Butane, 2,2,3,3-t...	6.34	281.2	ug/l	3689870	2	6.85	656132	50.0
Pentane, 2,3,4-tr...	8.05	114.3	ug/l	1499340	2	6.85	656132	50.0
Pentane, 2,3,3-tr...	8.17	154.6	ug/l	2028980	2	6.85	656132	50.0