

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX022819\
 Data File : VX007764.D
 Acq On : 28 Feb 2019 14:12
 Operator : JC/SP
 Sample : K1653-07
 Misc : 5.0mL/MSVOA X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-7

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\82X022519W.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	1.275	16	20	34	rBV	63340	108374	6.71%	0.997%
2	1.794	100	105	114	rVB	112908	160063	9.91%	1.473%
3	2.397	199	204	209	rBV2	13978	25894	1.60%	0.238%
4	2.848	270	278	282	rBV	41475	96448	5.97%	0.888%
5	2.891	282	285	289	rVV2	33786	66946	4.15%	0.616%
6	2.934	289	292	302	rVV	26353	52445	3.25%	0.483%
7	3.062	305	313	324	rVV	75521	175309	10.86%	1.613%
8	3.178	324	332	349	rVB2	63844	201260	12.46%	1.852%
9	4.305	504	517	524	rBV4	6405	23084	1.43%	0.212%
10	4.403	524	533	544	rVB	42170	123714	7.66%	1.139%
11	4.525	544	553	565	rVB6	4721	16712	1.03%	0.154%
12	5.269	671	675	687	rVB7	6543	20486	1.27%	0.189%
13	5.506	702	714	722	rBV	194493	568809	35.23%	5.235%
14	5.573	723	725	731	rVV2	32573	72901	4.51%	0.671%
15	5.665	731	740	768	rVB	317404	950656	58.87%	8.750%
16	5.933	773	784	796	rVV5	12050	43178	2.67%	0.397%
17	6.067	796	806	813	rVV	209701	536872	33.25%	4.941%
18	6.140	813	818	830	rVV	69695	195517	12.11%	1.799%
19	6.256	831	837	843	rVV5	14756	49729	3.08%	0.458%
20	6.354	847	853	862	rVV3	20936	64413	3.99%	0.593%
21	6.457	862	870	881	rVB4	17429	51535	3.19%	0.474%
22	6.860	925	936	947	rBV	494936	1156371	71.61%	10.643%
23	7.256	993	1001	1008	rBV2	17167	38070	2.36%	0.350%
24	7.451	1022	1033	1044	rVB5	19041	56189	3.48%	0.517%
25	8.055	1123	1132	1143	rVB4	6461	20268	1.26%	0.187%
26	8.177	1143	1152	1155	rBV3	10983	22687	1.40%	0.209%
27	8.573	1212	1217	1225	rVB7	11621	25641	1.59%	0.236%
28	8.713	1234	1240	1248	rVB	1070129	1614746	100.00%	14.862%
29	9.219	1318	1323	1334	rVB	19738	35225	2.18%	0.324%
30	9.512	1363	1371	1375	rBV3	11306	23734	1.47%	0.218%
31	10.109	1464	1469	1475	rVV	1028773	1386907	85.89%	12.765%
32	10.249	1488	1492	1496	rVB	21841	26933	1.67%	0.248%
33	11.018	1613	1618	1623	rBV	21883	30458	1.89%	0.280%
34	11.133	1632	1637	1643	rBV	859586	1109270	68.70%	10.209%

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Integration Parameters: RTEINT.P

Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

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Title : SW846 8260

35	11.359	1671	1674	1683	rVB	20513	28066	1.74%	0.258%
36	11.664	1719	1724	1733	rVB	47657	64873	4.02%	0.597%
37	12.078	1786	1792	1799	rBV	1050686	1316004	81.50%	12.112%
38	12.139	1799	1802	1814	rVB	14381	22866	1.42%	0.210%
39	12.298	1820	1828	1836	rBV2	68211	97164	6.02%	0.894%
40	12.517	1860	1864	1870	rVB	12960	16508	1.02%	0.152%
41	12.670	1884	1889	1891	rBV	15804	19519	1.21%	0.180%
42	12.755	1899	1903	1910	rVB2	24986	39990	2.48%	0.368%
43	12.975	1932	1939	1943	rBV	17956	24018	1.49%	0.221%
44	13.225	1977	1980	1983	rBV	17182	18887	1.17%	0.174%
45	13.346	1996	2000	2005	rBV	51359	66465	4.12%	0.612%

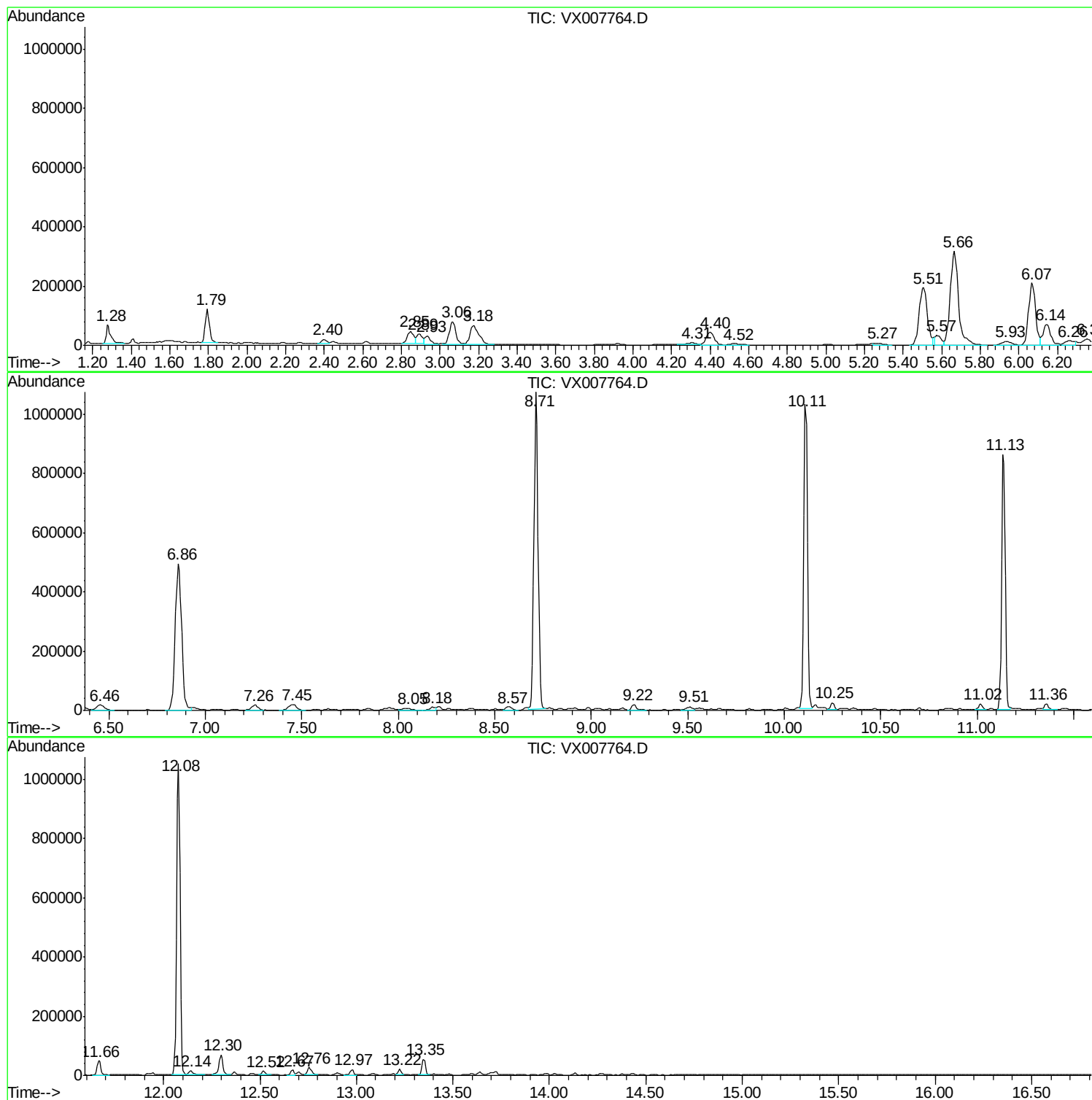
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Quant Title : SW846 8260

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



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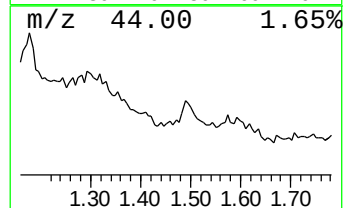
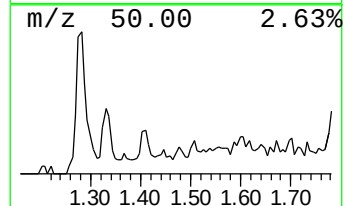
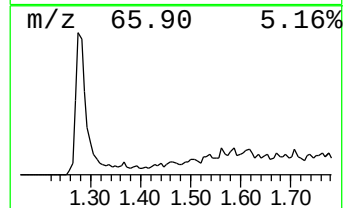
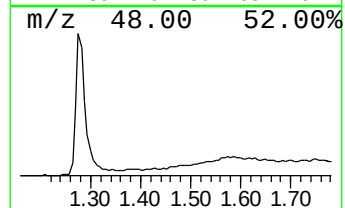
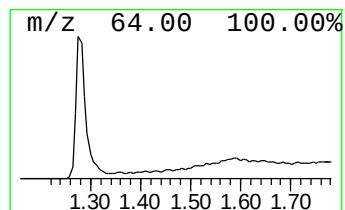
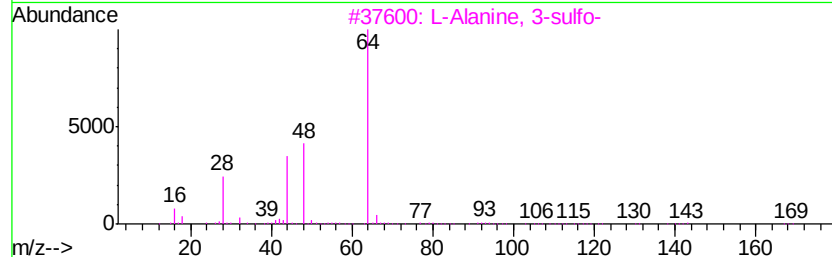
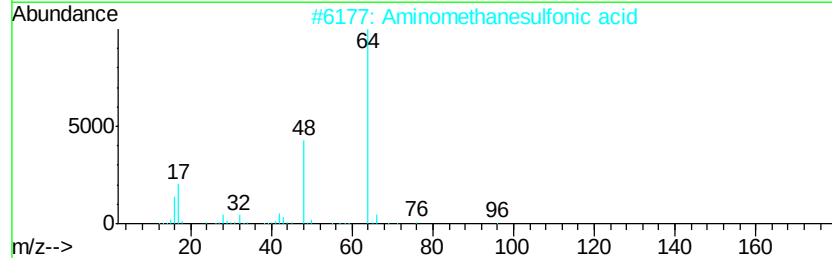
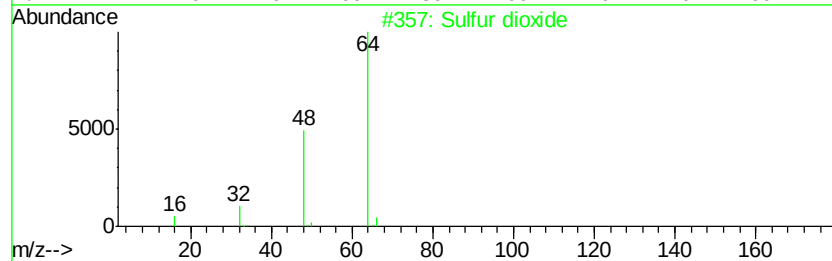
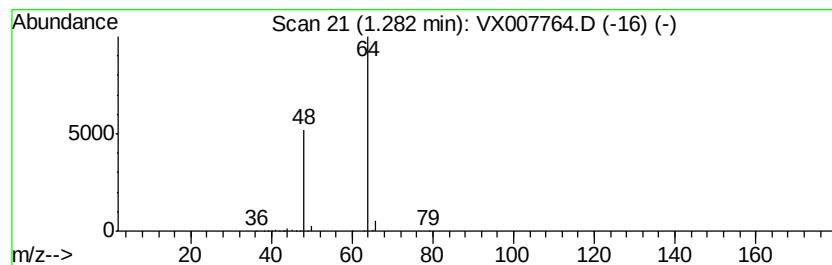
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X022519W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.28	5.70 ug/l	108374	Pentafluorobenzene	5.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide		64	O2S	007446-09-5	83
2	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	74
3	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,1-difluoro-		64	C2H2F2	000075-38-7	4
5	Ethyl Chloride		64	C2H5Cl	000075-00-3	3



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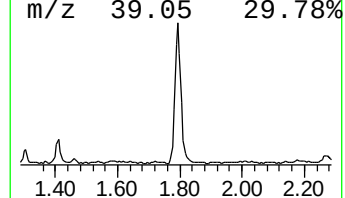
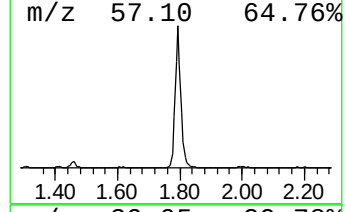
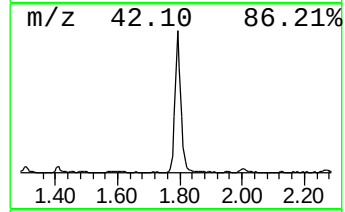
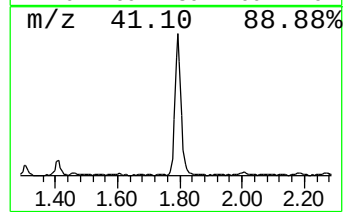
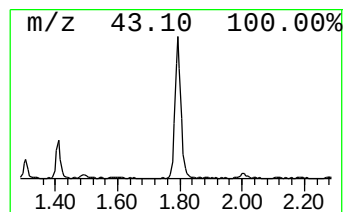
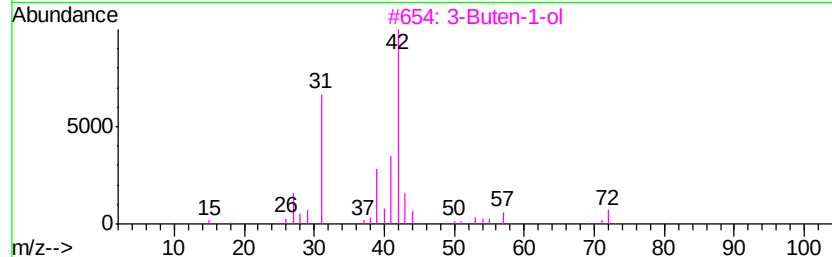
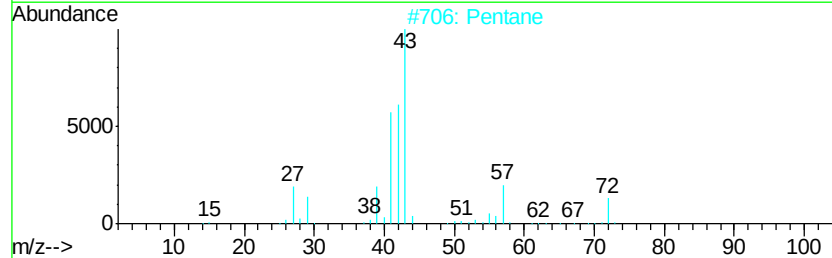
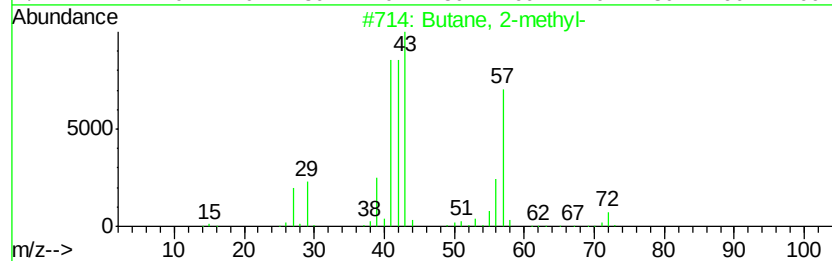
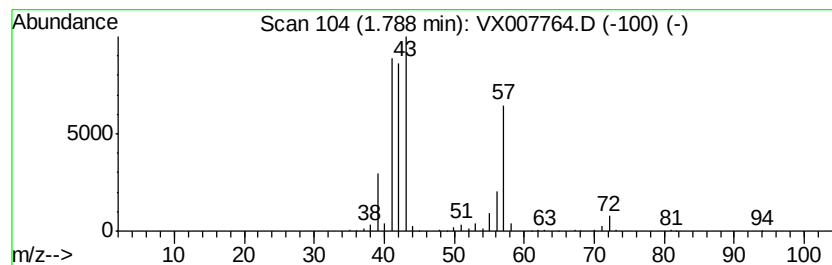
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	8.42 ug/l	160063	Pentafluorobenzene	5.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methyl-	72	C5H12	000078-78-4	91
2			Pentane	72	C5H12	000109-66-0	36
3			3-Buten-1-ol	72	C4H8O	000627-27-0	28
4			1-Butene	56	C4H8	000106-98-9	10
5			1-Propene, 2-methyl-	56	C4H8	000115-11-7	10



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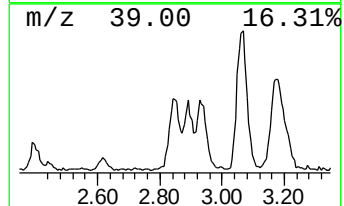
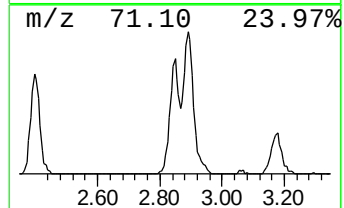
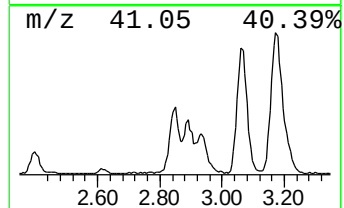
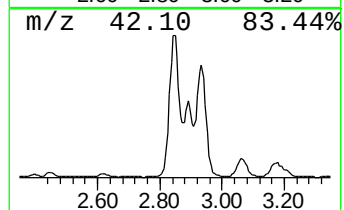
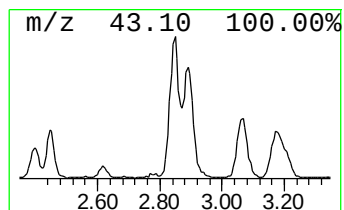
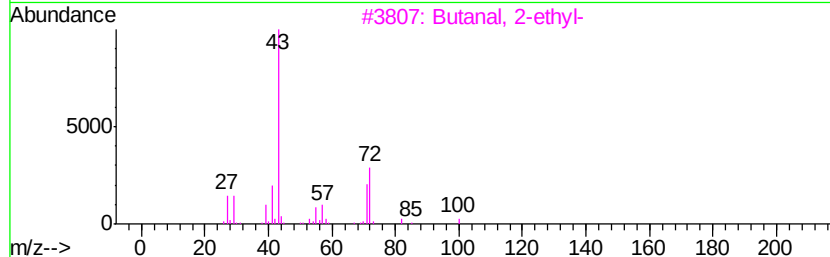
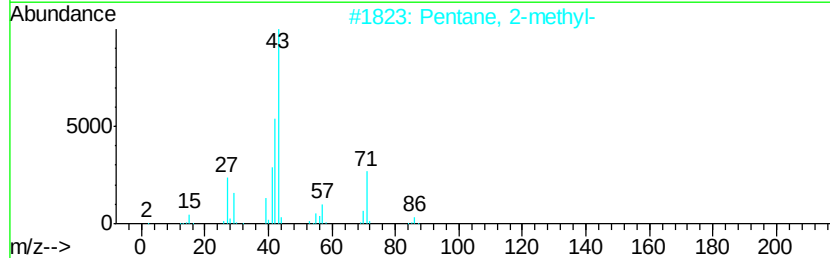
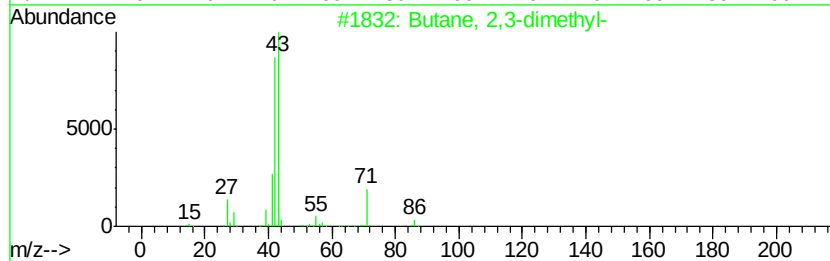
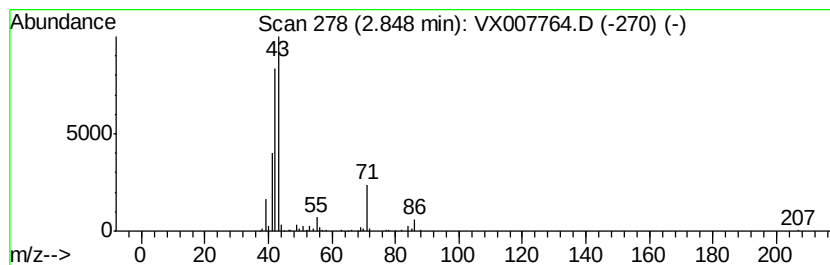
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X022519W.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	5.07 ug/l	96448	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2		Pentane, 2-methyl-	86	C6H14	000107-83-5	40
3		Butanal, 2-ethyl-	100	C6H12O	000097-96-1	10
4		Butanal, 2,2-dimethyl-	100	C6H12O	002094-75-9	9
5		C2H5C(CH3)2COCH3	114	C7H14O	020669-04-9	9



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ClientSampleId :
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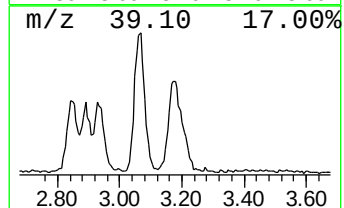
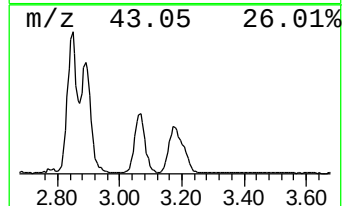
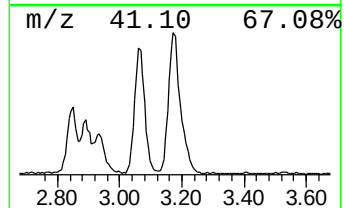
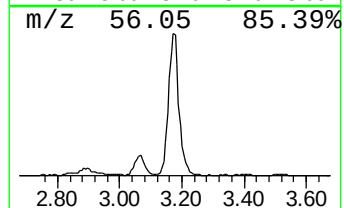
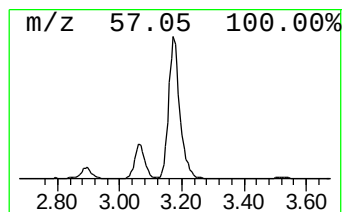
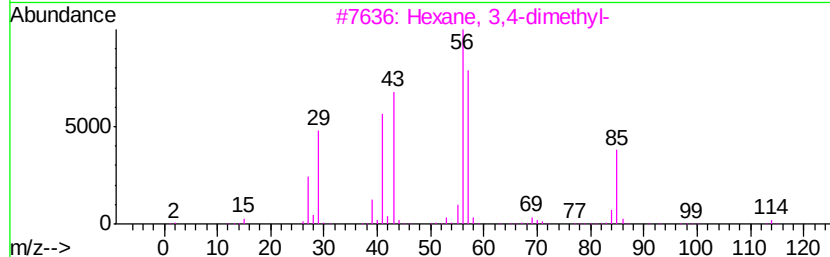
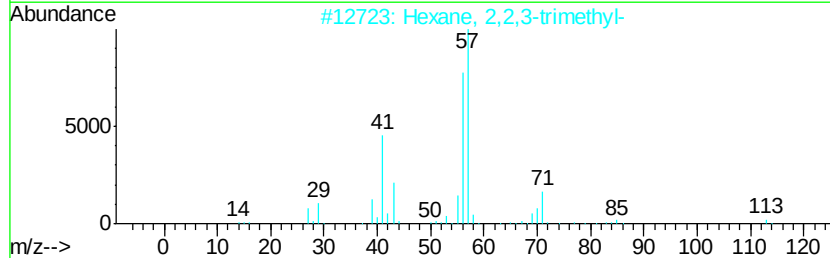
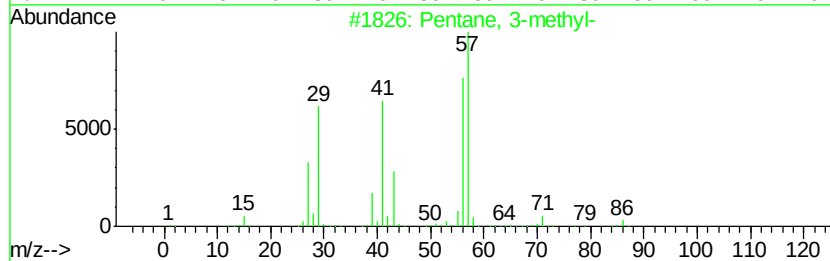
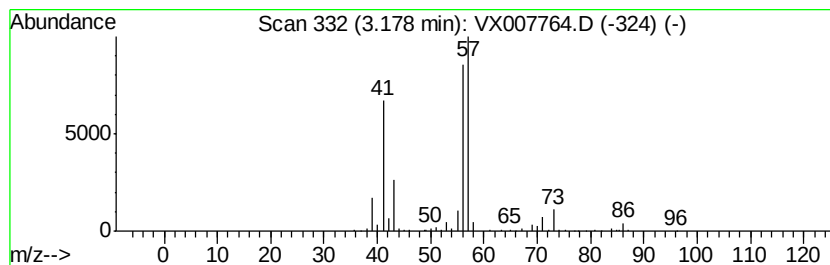
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Peak Number 4 Pentane, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	10.59 ug/l	201260	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentane, 3-methyl-	86	C6H14	000096-14-0	83
2		Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3		Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	64
4		Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	56
5		Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	53



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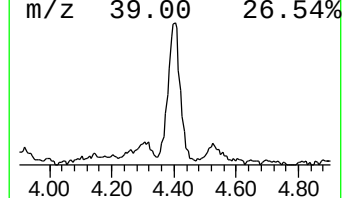
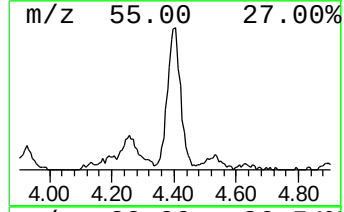
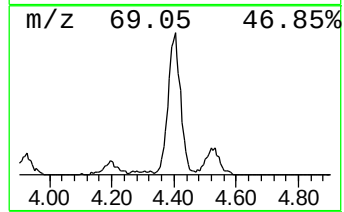
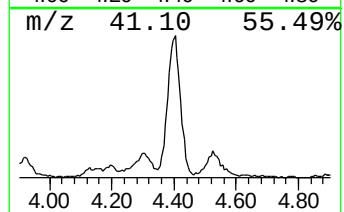
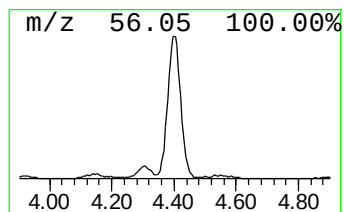
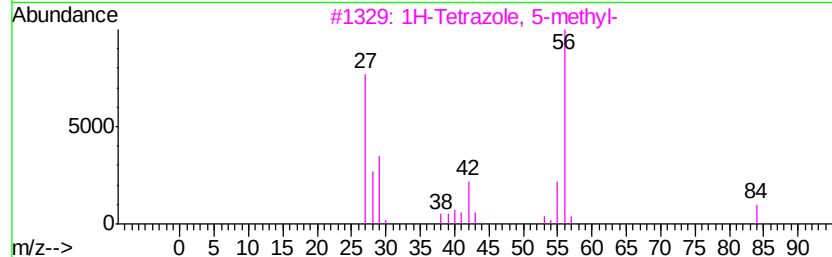
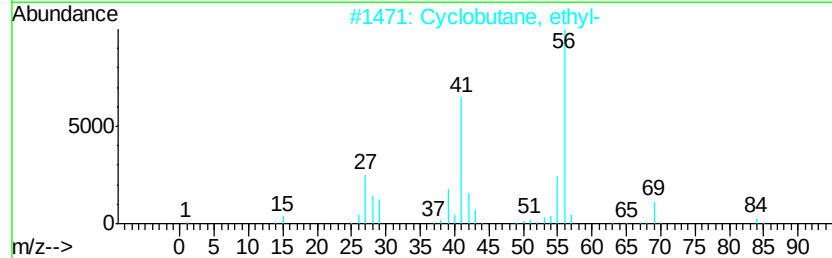
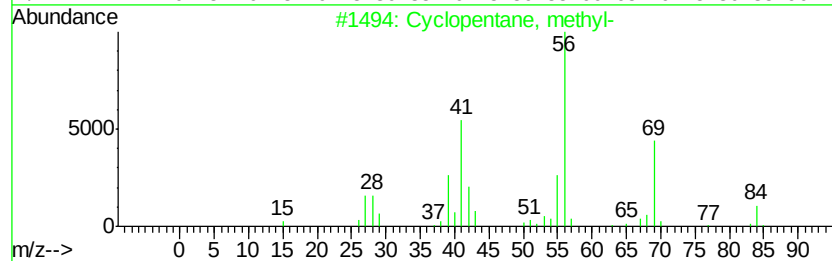
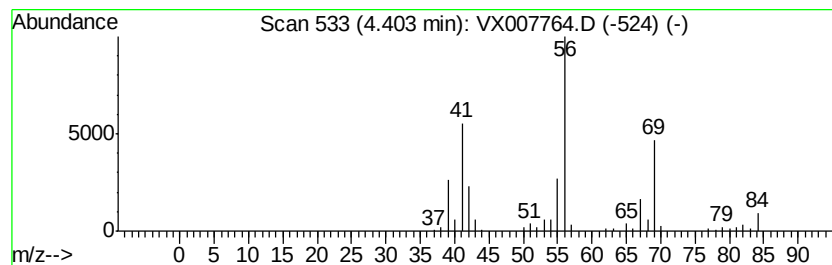
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TIC Integration Parameters: LSCINT.P

Peak Number 5 Cyclopentane, methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	6.51 ug/l	123714	Pentafluorobenzene	5.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentane, methyl-	84	C6H12	000096-37-7	74
2		Cyclobutane, ethyl-	84	C6H12	004806-61-5	53
3		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	53
4		1-Pentene, 2-methyl-	84	C6H12	000763-29-1	45
5		Cyclobutane	56	C4H8	000287-23-0	43



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_X\DATA\VX022819\
Data File : VX007764.D
Acq On : 28 Feb 2019 14:12
Operator : JC/SP
Sample : K1653-07
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-7

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_X\METHOD\82X022519W.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
Sulfur dioxide	1.28	5.7	ug/l	108374	1	5.66	950656	50.0
Butane, 2-methyl-	1.79	8.4	ug/l	160063	1	5.66	950656	50.0
Butane, 2,3-dimet...	2.85	5.1	ug/l	96448	1	5.66	950656	50.0
Pentane, 3-methyl-	3.18	10.6	ug/l	201260	1	5.66	950656	50.0
Cyclopentane, met...	4.40	6.5	ug/l	123714	1	5.66	950656	50.0