LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.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	1.794	99	105	117	rVB	614816	908885	4.93%	0.570%
2	2.001	133	139	152	rVB	913255	1287601	6.99%	0.808%
3	2.398	195	204	217	rBV	188819	391231	2.12%	0.245%
4	2.849	269	278	280	rBV	328524	657275	3.57%	0.412%
5	2.891	280	285	303	rVB	1233082	2780117	15.09%	1.744%
6	3.178	321	332	349	rBV	1015380	2361582	12.82%	1.481%
7	3.525	377	389	406	rBV	1168628	2675487	14.52%	1.678%
8	4.409	523	534	549	rVB	2521786	7414216	40.24%	4.651%
9	5.501	699	713	716	rBV	134881	351919	1.91%	0.221%
10	5.586	716	727	737	rBV	2414041	7500380	40.71%	4.705%
11	5.726	746	750	767	rVB	123281	355499	1.93%	0.223%
12	5.940	770	785	797	rBV5	359208	1237162	6.71%	0.776%
13	6.062	797	805	820	rVV	135157	354378	1.92%	0.222%
14	6.263	824	838	847	rVV2	244343	755390	4.10%	0.474%
15	6.360	847	854	862	rVV2	241238	652958	3.54%	0.410%
16	6.458	862	870	883	rVB	346004	957990	5.20%	0.601%
17	6.860	926	936	946	rBV	349822	839258	4.55%	0.526%
18	7.464	1021	1035	1047	rBV	3406413	7692212	41.75%	4.825%
19	7.732	1071	1079	1090	rVB	225391	439111	2.38%	0.275%
20	8.665	1225	1232	1235	rBV	346946	595753	3.23%	0.374%
21	8.714	1235	1240	1246	rVB	797769	1373077	7.45%	0.861%
22	8.781	1246	1251	1256	rBV	577357	881012	4.78%	0.553%
23	8.835	1256	1260	1265	rVB	134582	208951	1.13%	0.131%
24	9.037	1288	1293	1300	rVB	262948	417523	2.27%	0.262%
25	9.165	1305	1314	1319	rBV	202267	326358	1.77%	0.205%
26	9.622	1385	1389	1394	rVB	330784	451555	2.45%	0.283%
27	10.110	1464	1469	1475	rBV	774196	999231	5.42%	0.627%
28	10.183	1475	1481	1486	rBV	182939	254916	1.38%	0.160%
29	10.250	1486	1492	1498	rBV	3482846	4453027	24.17%	2.793%
30	10.360	1501	1510	1516	rBV	13403121	18085922	98.16%	11.345%
31	10.695	1560	1565	1576	rVB	3364501	4322743	23.46%	2.712%
32	11.018	1612	1618	1629	rVB	1297825	1649747	8.95%	1.035%
33	11.134	1632	1637	1642	rBV	702254	879441	4.77%	0.552%
34	11.359	1664	1674	1681	rBV	2110697	2582237	14.01%	1.620%

LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Title : SW846 8260

35	11.433	1681	1686	1694	rVV	9171992	16036371	87.03%	10.059%
36	11.506	1694	1698	1703	rVB	6735174	7934309	43.06%	4.977%
37	11.664	1719	1724	1732	rBV	3908967	4860984	26.38%	3.049%
38	11.768	1734	1741	1743	rBV	152146	209368	1.14%	0.131%
39	11.811	1743	1748	1753	rVB	14686013	18425733	100.00%	11.558%
40	11.920	1760	1766	1768	rBV	143523	209306	1.14%	0.131%
41	11.945	1768	1770	1777	rVB	196197	204243	1.11%	0.128%
42	12.024	1777	1783	1786	rBV	447061	542414	2.94%	0.340%
43	12.073	1786	1791	1797	rVB2	976487	1402686	7.61%	0.880%
44	12.140	1797	1802	1808	rBV	5409300	6544134	35.52%	4.105%
45	12.298	1822	1828	1831	rBV	2115716	2982260	16.19%	1.871%
46	12.371	1835	1840	1849	rVB3	1563704	2300377	12.48%	1.443%
47	12.518	1859	1864	1869	rBV	390749	468150	2.54%	0.294%
48	12.585	1870	1875	1877	rBV	749603	993947	5.39%	0.623%
49	12.609	1877	1879	1883	rVV	772928	783453	4.25%	0.491%
50	12.664	1883	1888	1891	rVV	1043776	1210773	6.57%	0.759%
51	12.701	1891	1894	1898	rVV	331231	384707	2.09%	0.241%
52	12.756	1898	1903	1911	rVV3	703884	1200623	6.52%	0.753%
53	12.902	1922	1927	1932	rVB2	475805	617284	3.35%	0.387%
54	12.975	1932	1939	1942	rBV	621542	767251	4.16%	0.481%
55	13.018	1942	1946	1951	rVB	901112	1073016	5.82%	0.673%
56	13.225	1972	1980	1984	rBV	951968	1244372	6.75%	0.781%
57	13.347	1995	2000	2005	rVB2	2105423	2809364	15.25%	1.762%
58	13.475	2016	2021	2027	rVB	1443908	1782185	9.67%	1.118%
59	13.639	2044	2048	2052	rBV3	145791	237326	1.29%	0.149%
60	13.719	2058	2061	2067	rVB2	141399	221765	1.20%	0.139%
61	13.828	2071	2079	2087	rVV	1781336	2364899	12.83%	1.483%
62	13.981	2097	2104	2108	rBV2	140076	206620	1.12%	0.130%
63	14.286	2146	2154	2161	rVB2	247133	452780	2.46%	0.284%
64	14.536	2190	2195	2200	rBV2	156655	207809	1.13%	0.130%
65	14.694	2213	2221	2226	rBV	1753462	2098471	11.39%	1.316%
66	14.834	2239	2244	2253	rBV	1104933	1354822	7.35%	0.850%
67	15.682	2375	2383	2387	rBV	114485	194986	1.06%	0.122%

Sum of corrected areas: 159420932

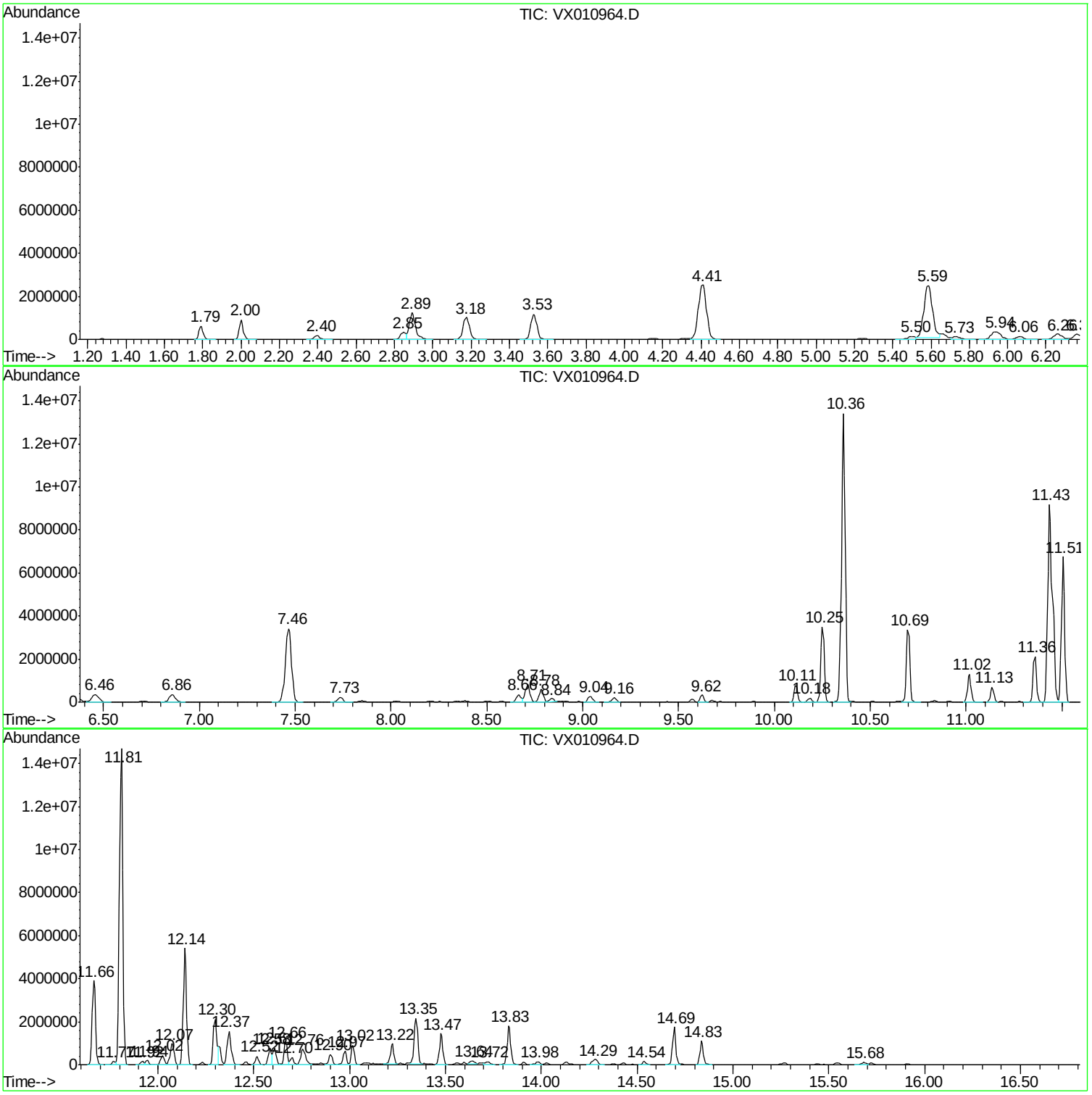
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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



Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

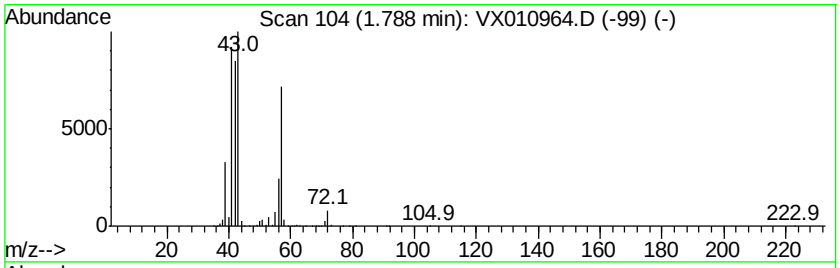
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

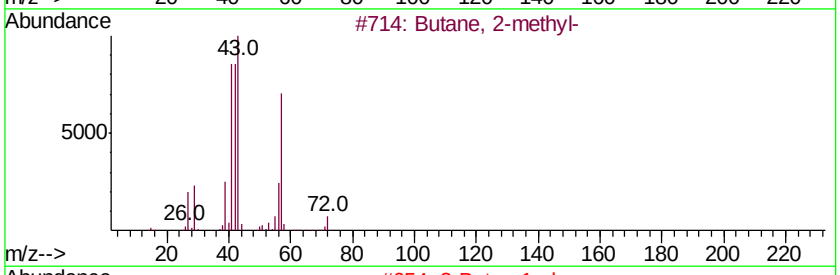
****

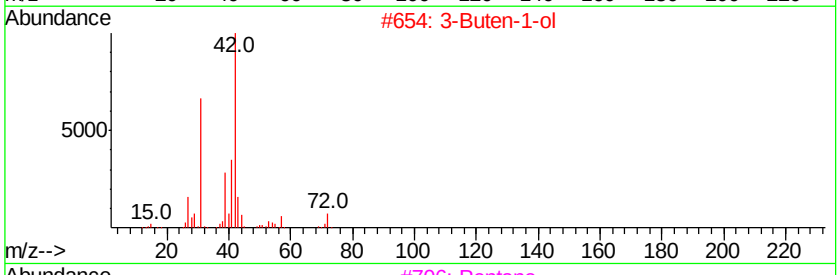
Peak Number 1 Butane, 2-methyl- Concentration Rank 10

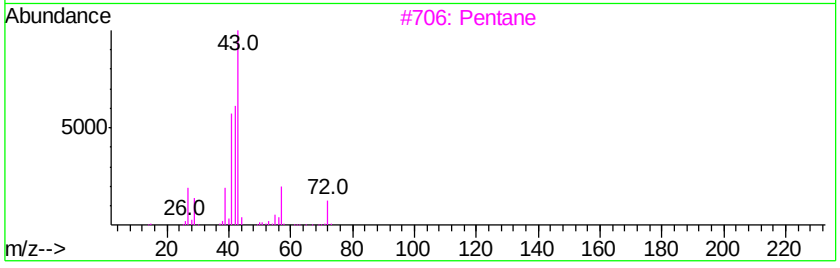
R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	127.83 ug/l	908885	Pentafluorobenzene	5.67

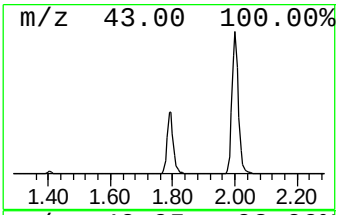
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	3-Buten-1-ol	72	C4H8O	000627-27-0	38
3	Pentane	72	C5H12	000109-66-0	36
4	1-Butene	56	C4H8	000106-98-9	14
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10

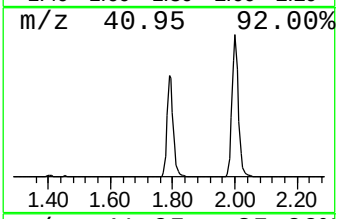


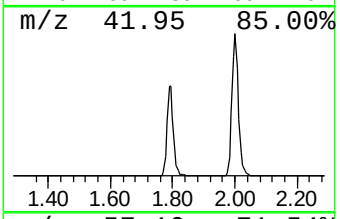


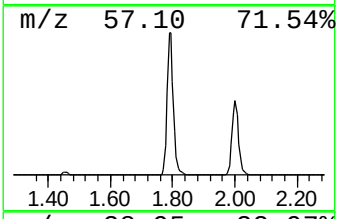


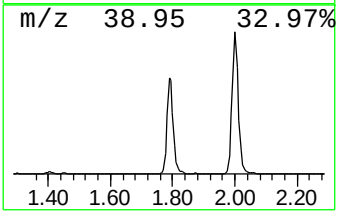












Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

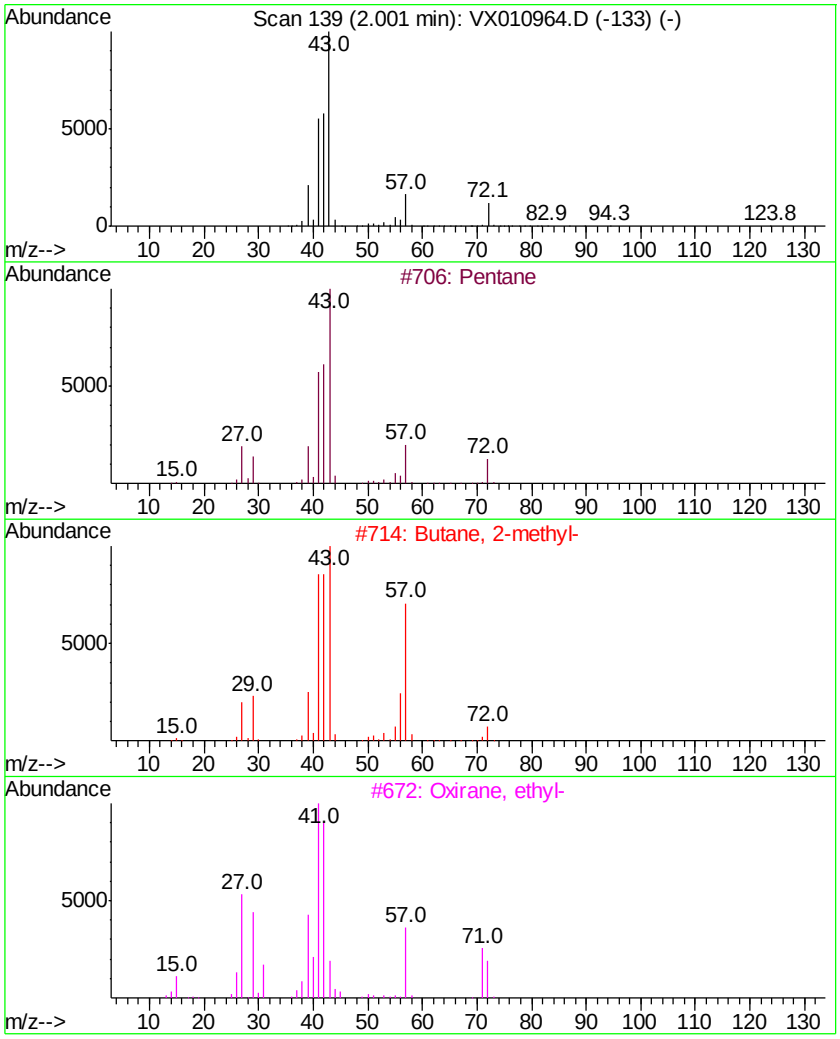
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

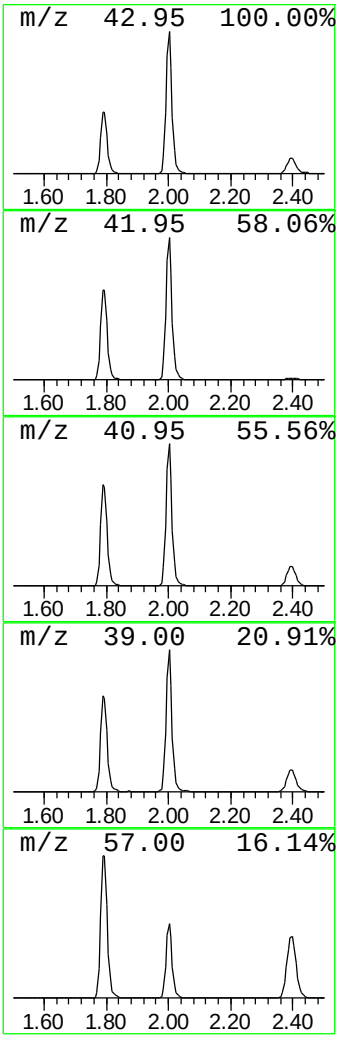
****

Peak Number 2 Pentane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	181.10 ug/l	1287600	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Butane, 2-methyl-	72	C5H12	000078-78-4	53
3	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	2(3H)-Furanone, dihydro-4-methyl-	100	C5H8O2	001679-49-8	25





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

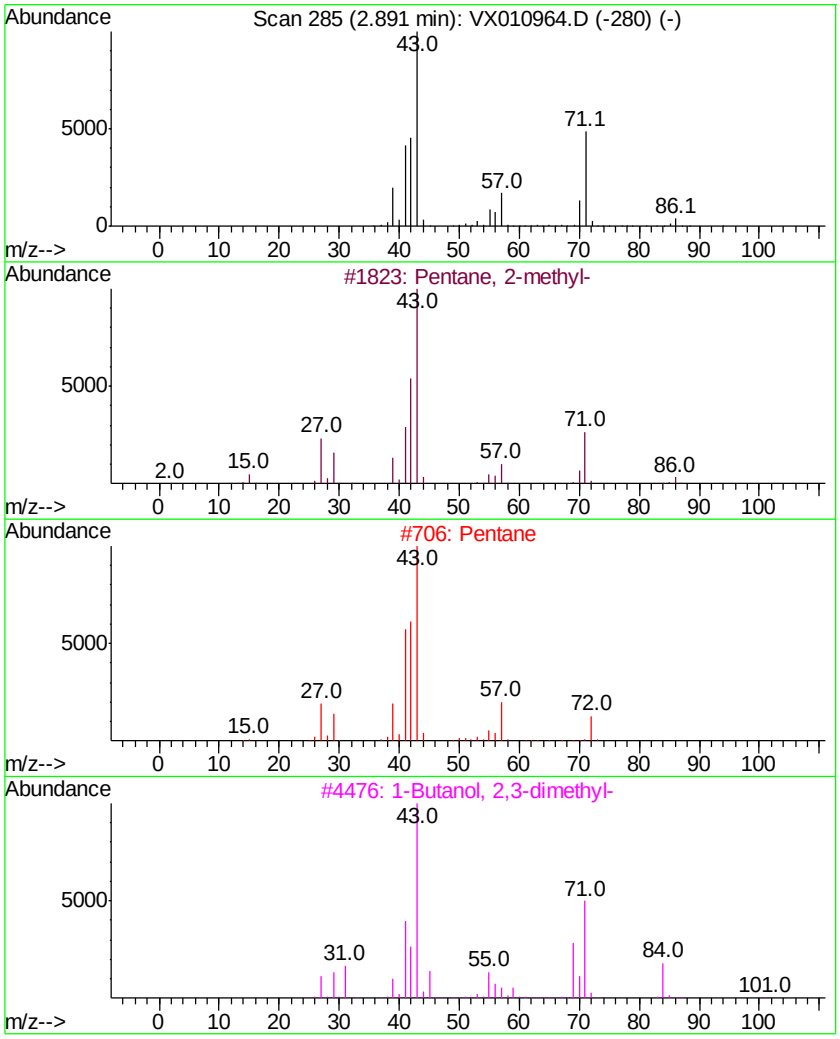
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

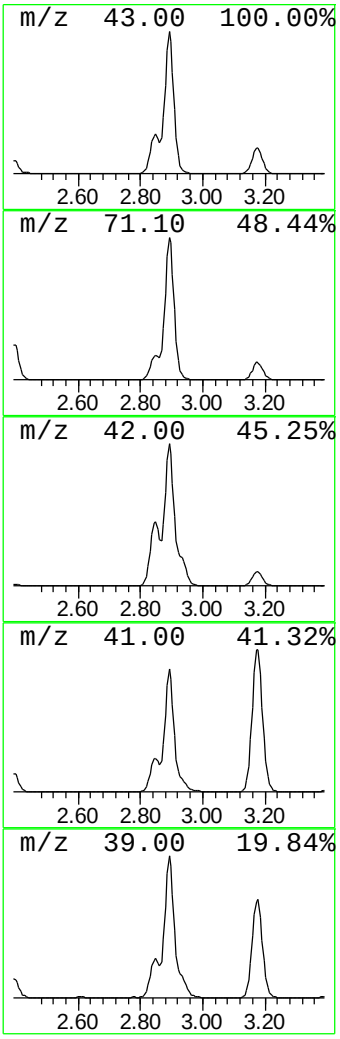
****

Peak Number 3 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	391.02 ug/l	2780120	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2	Pentane	72	C5H12	000109-66-0	46
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
4	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	43
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

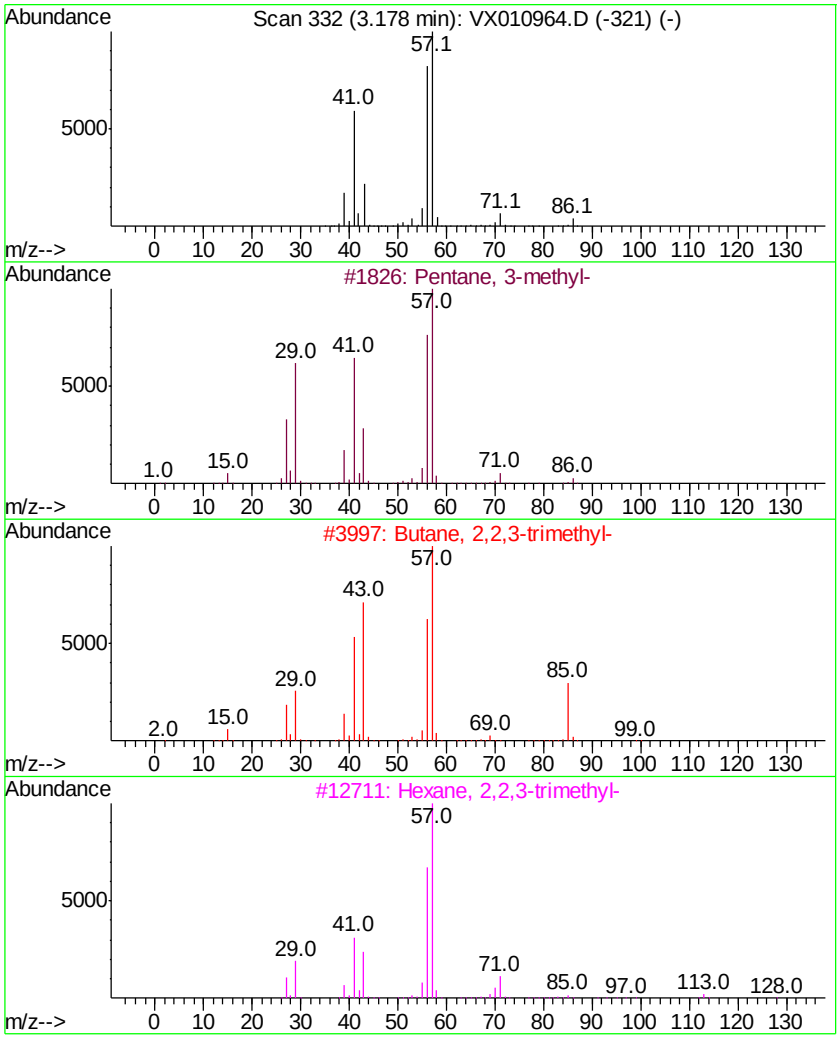
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

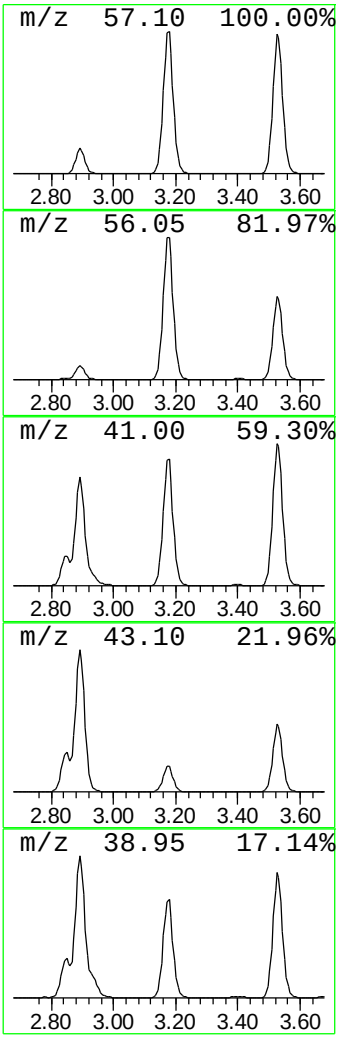
****

Peak Number 4 Pentane, 3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	332.15 ug/l	2361580	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	64
3	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

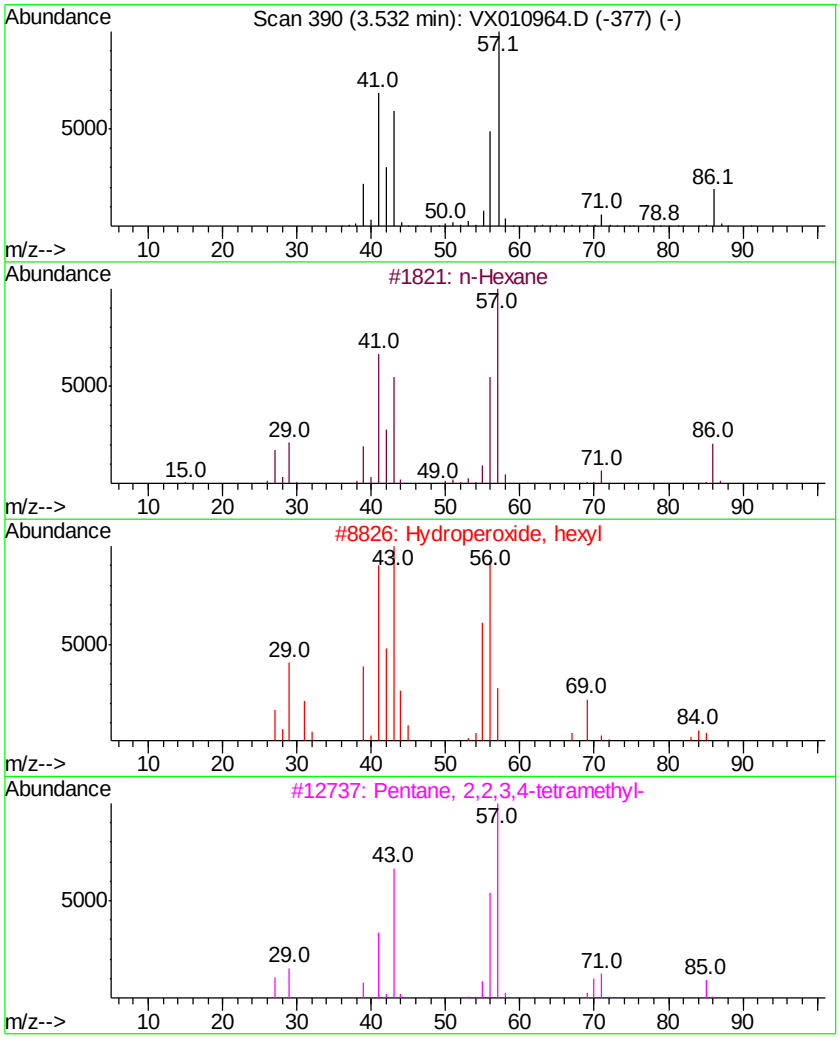
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

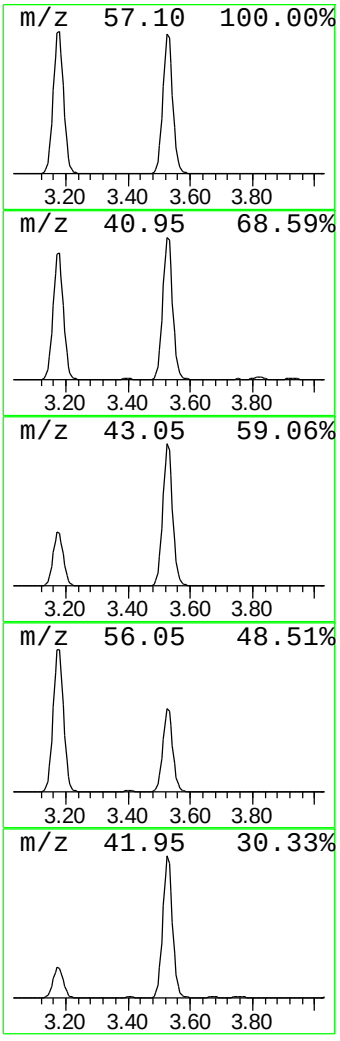
****

Peak Number 5 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	376.30 ug/l	2675490	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	94
2	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	47
3	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	42
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

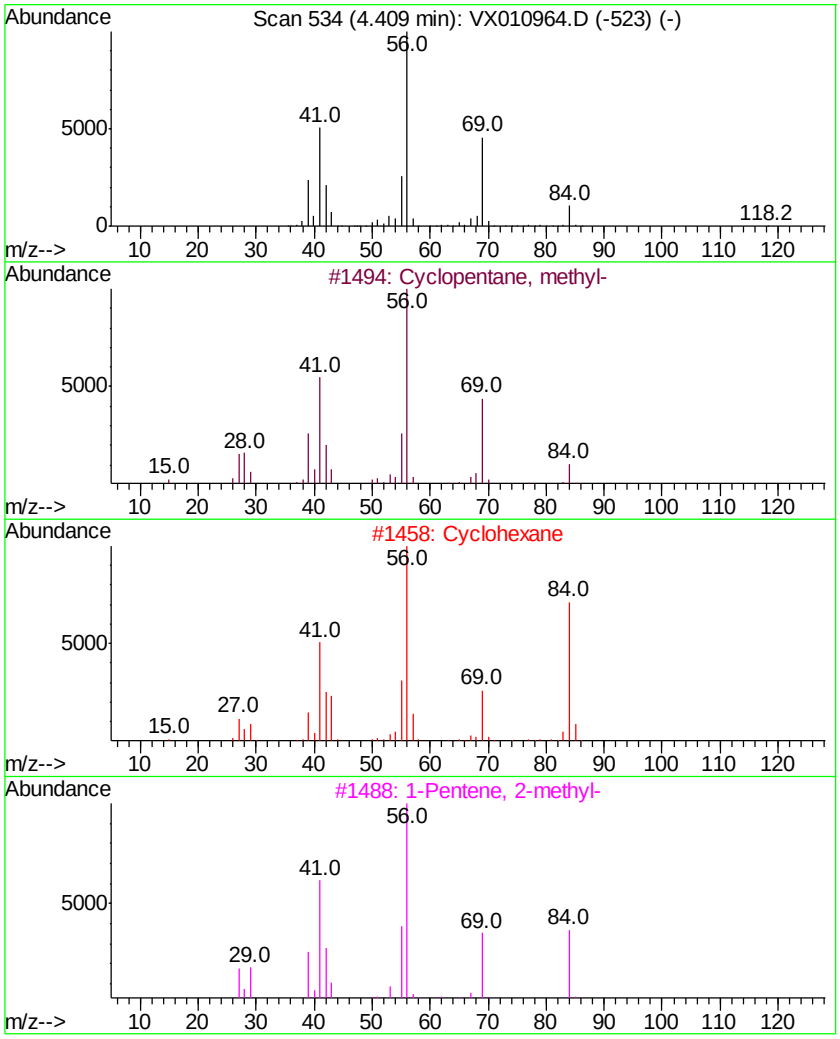
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

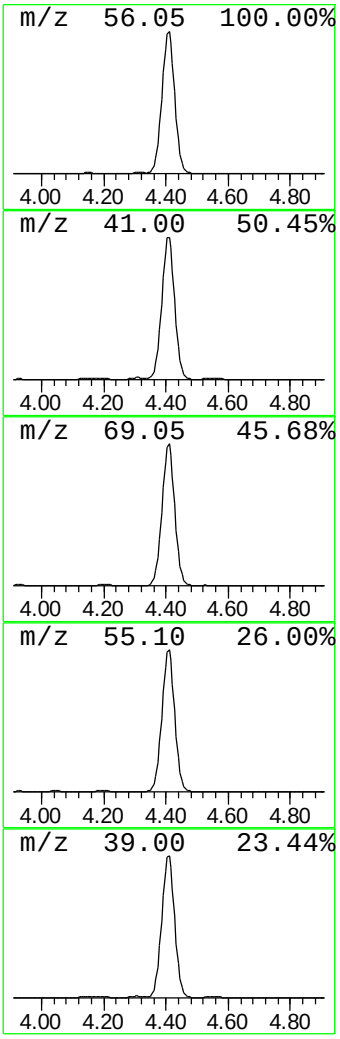
****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	1042.79 ug/l	7414220	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	59





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

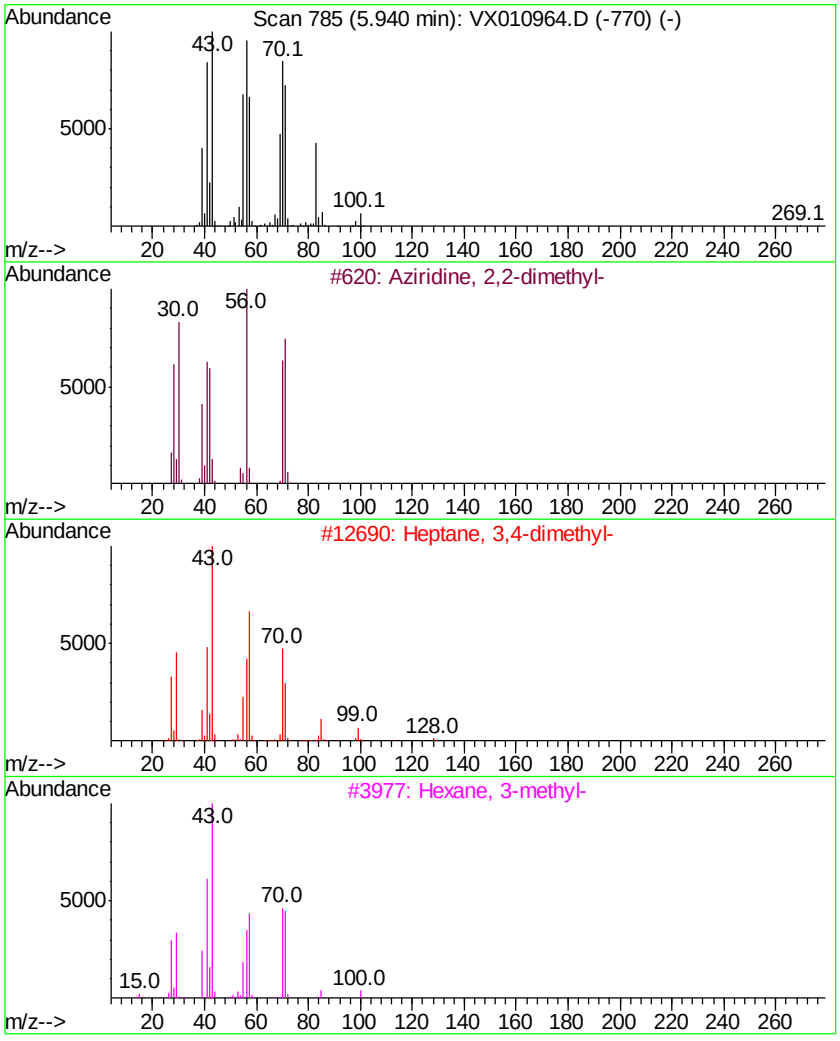
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

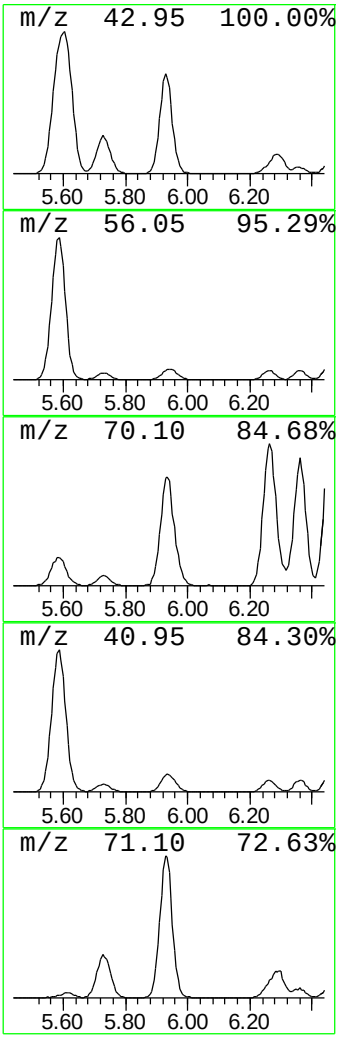
****

Peak Number 7 Aziridine, 2,2-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.94	174.00 ug/l	1237160	Pentafluorobenzene	5.67

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aziridine, 2,2-dimethyl-	71	C4H9N	002658-24-4	59
2	Heptane, 3,4-dimethyl-	128	C9H20	000922-28-1	53
3	Hexane, 3-methyl-	100	C7H16	000589-34-4	53
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	47
5	Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	38





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

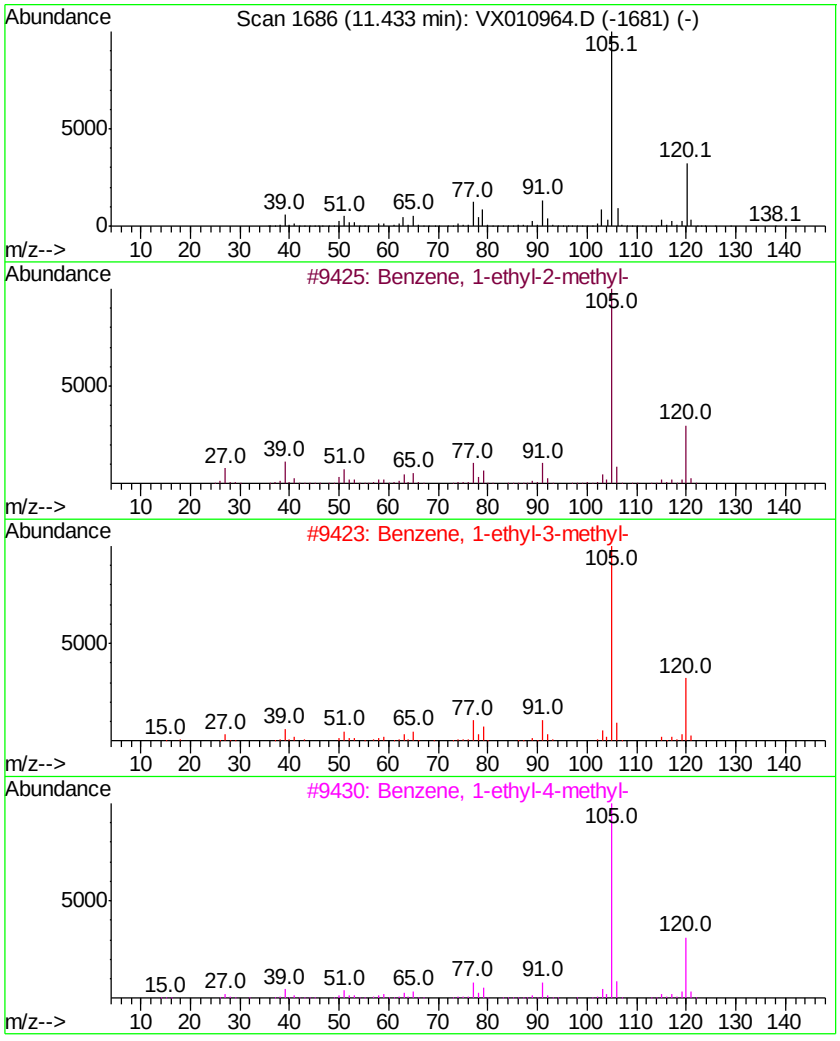
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

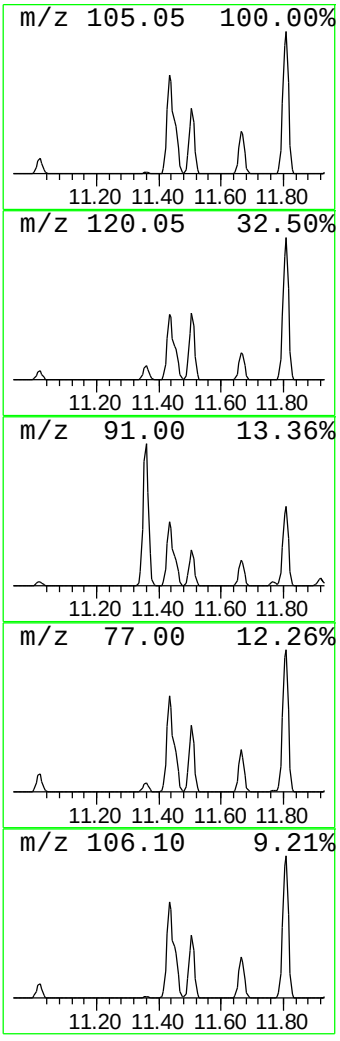
****

Peak Number 8 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	571.63 ug/l	16036400	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

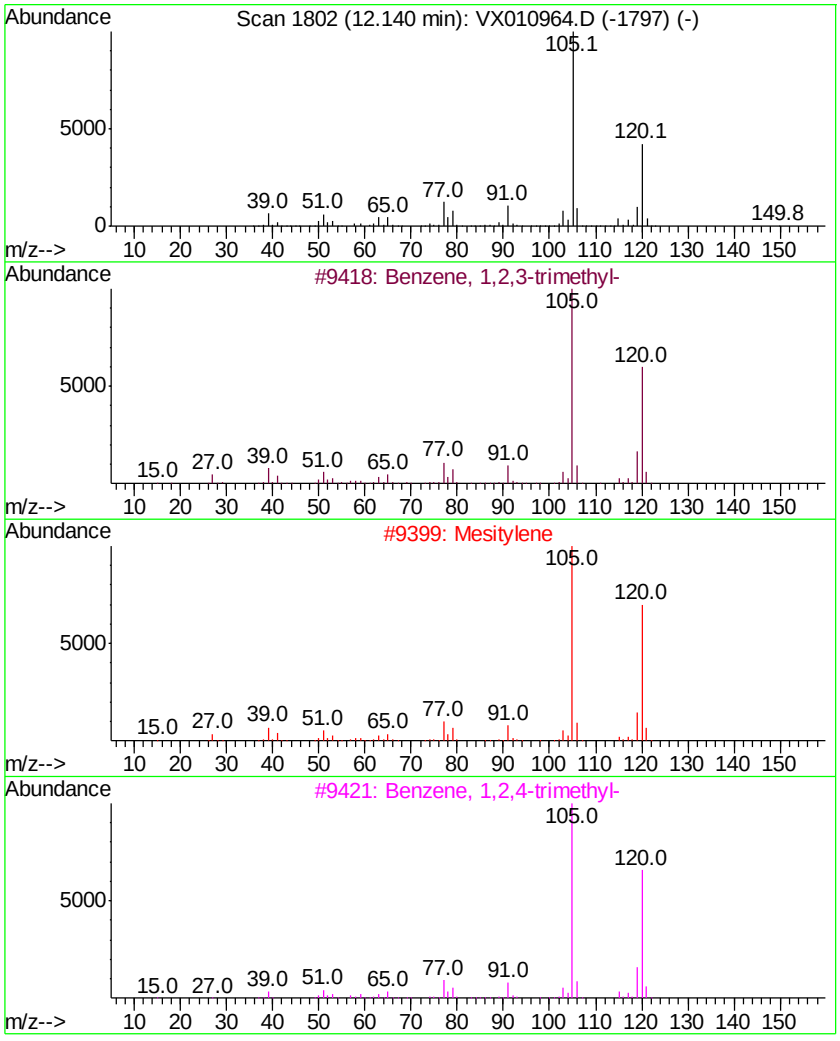
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

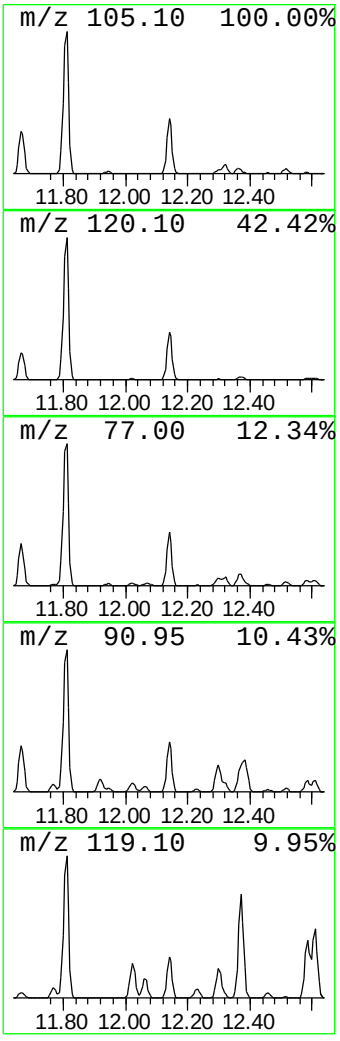
****

Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	233.27 ug/l	6544130	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
2	Mesitylene	120	C9H12	000108-67-8	91
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010964.D
Acq On : 18 Jul 2019 17:19
Operator : JC/SP
Sample : K3884-04
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0606

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_X\METHOD\82X071619W.M
Quant Title : SW846 8260

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	1.79	127.8	ug/l	908885	1	5.67	355499	50.0
Pentane	2.00	181.1	ug/l	1287600	1	5.67	355499	50.0
Pentane, 2-methyl-	2.89	391.0	ug/l	2780120	1	5.67	355499	50.0
Pentane, 3-methyl-	3.18	332.1	ug/l	2361580	1	5.67	355499	50.0
n-Hexane	3.53	376.3	ug/l	2675490	1	5.67	355499	50.0
Cyclopentane, met...	4.41	1042.8	ug/l	7414220	1	5.67	355499	50.0
Aziridine, 2,2-di...	5.94	174.0	ug/l	1237160	1	5.67	355499	50.0
Benzene, 1-ethyl-...	11.43	571.6	ug/l	16036400	4	12.08	1402690	50.0
Benzene, 1,2,3-tr...	12.14	233.3	ug/l	6544130	4	12.08	1402690	50.0