LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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	1.403	38	41	46	rBV	134478	133025	1.30%	0.185%
2	1.794	99	105	118	rVB	555487	798762	7.78%	1.109%
3	2.001	134	139	150	rVB	458748	642573	6.26%	0.892%
4	2.397	193	204	217	rVB	59107	126270	1.23%	0.175%
5	2.848	270	278	280	rBV	87169	172254	1.68%	0.239%
6	2.891	280	285	289	rVV	339896	725522	7.07%	1.008%
7	2.934	289	292	304	rVB	193622	369146	3.60%	0.513%
8	3.178	321	332	345	rBV	302483	702241	6.84%	0.975%
9	3.525	378	389	405	rBV	285639	651803	6.35%	0.905%
10	4.409	523	534	547	rVB	740275	2184904	21.29%	3.034%
11	5.500	697	713	718	rBV	131729	376986	3.67%	0.524%
12	5.586	718	727	735	rVV2	545300	1787201	17.41%	2.482%
13	5.659	735	739	747	rVB	178201	438679	4.27%	0.609%
14	5.933	770	784	797	rBV5	195492	651017	6.34%	0.904%
15	6.061	797	805	816	rVB	129062	333435	3.25%	0.463%
16	6.262	827	838	847	rBV2	114576	369018	3.60%	0.512%
17	6.360	847	854	862	rVV2	112477	314017	3.06%	0.436%
18	6.457	862	870	882	rVB	170120	474531	4.62%	0.659%
19	6.707	901	911	922	rBV	79786	190468	1.86%	0.265%
20	6.860	927	936	945	rBV	328553	789061	7.69%	1.096%
21	7.463	1022	1035	1047	rBV	1258115	2848284	27.75%	3.956%
22	7.732	1070	1079	1088	rVB	123366	246265	2.40%	0.342%
23	7.847	1088	1098	1106	rVB2	54621	112623	1.10%	0.156%
24	8.664	1225	1232	1235	rBV	201660	349407	3.40%	0.485%
25	8.713	1235	1240	1250	rVB	741738	1233286	12.02%	1.713%
26	8.841	1254	1261	1265	rBV	86756	150383	1.47%	0.209%
27	9.036	1288	1293	1300	rVB	158658	263119	2.56%	0.365%
28	9.164	1305	1314	1320	rBV	104040	169390	1.65%	0.235%
29	9.573	1374	1381	1385	rBV3	75338	136840	1.33%	0.190%
30	9.622	1385	1389	1394	rVB	202298	270512	2.64%	0.376%
31	9.676	1394	1398	1402	rBV	78937	112610	1.10%	0.156%
32	10.109	1464	1469	1476	rVB	713050	944075	9.20%	1.311%
33	10.182	1476	1481	1486	rVB	80357	115993	1.13%	0.161%
34	10.249	1486	1492	1498	rBV	3539428	4596906	44.79%	6.384%

LSC Area Percent Report

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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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	10.359	1501	1510	1516	rBV	7657977	10262847	100.00%	14.253%
36	10.701	1560	1566	1577	rVB	3657188	4885000	47.60%	6.784%
37	11.018	1612	1618	1623	rBV	538362	665330	6.48%	0.924%
38	11.133	1632	1637	1642	rBV	656323	830386	8.09%	1.153%
39	11.359	1669	1674	1681	rBV	713919	858361	8.36%	1.192%
40	11.432	1681	1686	1693	rVV	2375119	4188947	40.82%	5.818%
41	11.505	1693	1698	1707	rVB	1771744	2118815	20.65%	2.943%
42	11.664	1719	1724	1732	rBV	1206283	1479824	14.42%	2.055%
43	11.804	1742	1747	1752	rVB	4180834	5039680	49.11%	6.999%
44	11.944	1767	1770	1776	rVB	128830	163684	1.59%	0.227%
45	12.024	1776	1783	1786	rBV	274665	333376	3.25%	0.463%
46	12.072	1786	1791	1797	rVB2	850427	1214054	11.83%	1.686%
47	12.139	1797	1802	1808	rBV	1752921	2050014	19.98%	2.847%
48	12.298	1822	1828	1830	rBV	643172	820295	7.99%	1.139%
49	12.322	1830	1832	1835	rVV	399913	399888	3.90%	0.555%
50	12.371	1835	1840	1848	rVB3	638111	965852	9.41%	1.341%
51	12.456	1849	1854	1859	rBV	81106	102706	1.00%	0.143%
52	12.517	1859	1864	1869	rVB	242431	291371	2.84%	0.405%
53	12.584	1869	1875	1877	rBV	339299	448091	4.37%	0.622%
54	12.609	1877	1879	1883	rVB	405396	399173	3.89%	0.554%
55	12.664	1883	1888	1892	rBV	507269	587371	5.72%	0.816%
56	12.700	1892	1894	1899	rVB	108180	117600	1.15%	0.163%
57	12.761	1899	1904	1911	rBV3	281041	591846	5.77%	0.822%
58	12.901	1922	1927	1931	rVB2	289289	380289	3.71%	0.528%
59	12.975	1931	1939	1942	rBV	363211	461216	4.49%	0.641%
60	13.017	1942	1946	1952	rVB	546586	657174	6.40%	0.913%
61	13.078	1952	1956	1961	rBV2	93730	185914	1.81%	0.258%
62	13.225	1972	1980	1983	rBV3	189505	314676	3.07%	0.437%
63	13.340	1995	1999	2005	rVB2	858015	1218326	11.87%	1.692%
64	13.474	2016	2021	2030	rVB	534174	733273	7.14%	1.018%
65	13.633	2044	2047	2053	rBV4	130033	231106	2.25%	0.321%
66	13.718	2059	2061	2067	rVB2	110669	165363	1.61%	0.230%
67	13.834	2071	2080	2087	rVV	1199790	1632410	15.91%	2.267%
68	13.907	2088	2092	2097	rVB	109421	143336	1.40%	0.199%
69	13.987	2097	2105	2109	rBV2	128302	221327	2.16%	0.307%
70	14.285	2146	2154	2160	rVB2	211845	367725	3.58%	0.511%
71	14.535	2190	2195	2204	rBV2	172117	233714	2.28%	0.325%

LSC Area Percent Report

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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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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Peak separation: 5

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

72	14.694	2214	2221	2225	rBV	911439	1128801	11.00%	1.568%
73	14.834	2239	2244	2249	rBV	584836	758448	7.39%	1.053%
74	15.267	2307	2315	2320	rVB2	54752	113902	1.11%	0.158%
75	15.547	2353	2361	2366	rBV	94884	160043	1.56%	0.222%
76	15.681	2376	2383	2387	rBV	111378	187251	1.82%	0.260%
77	15.724	2387	2390	2397	rVB	79917	116445	1.13%	0.162%

Sum of corrected areas: 72005856

LSC Report - Integrated Chromatogram

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Data File : VX010963.D
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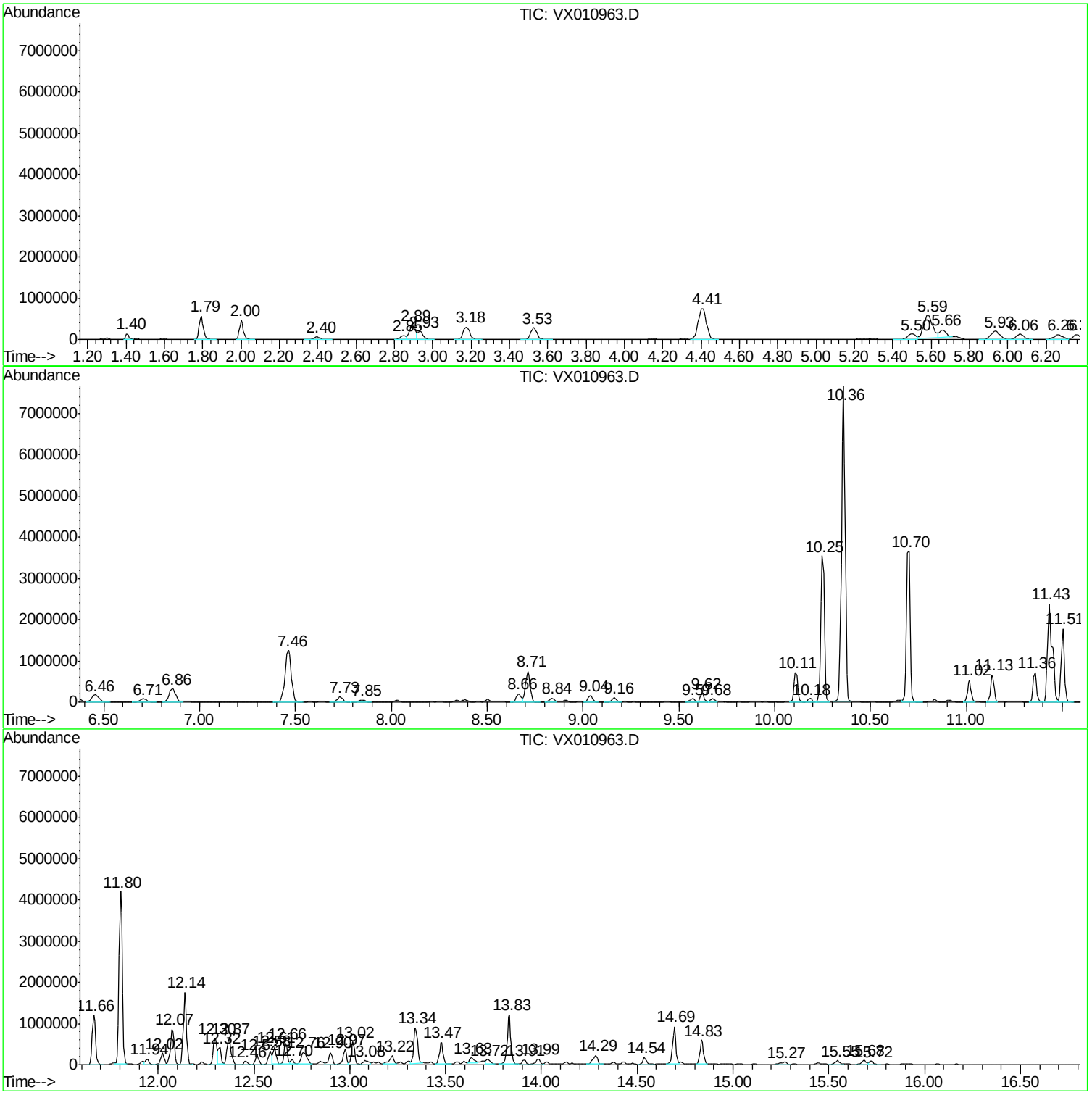
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

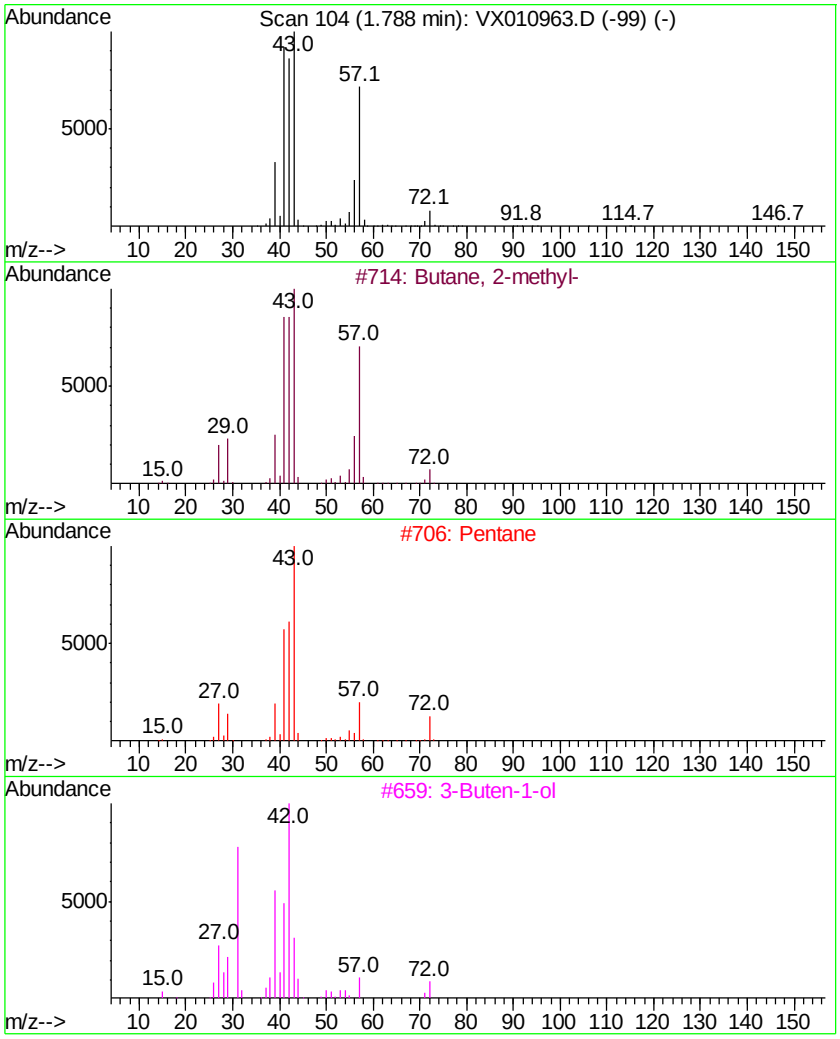
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

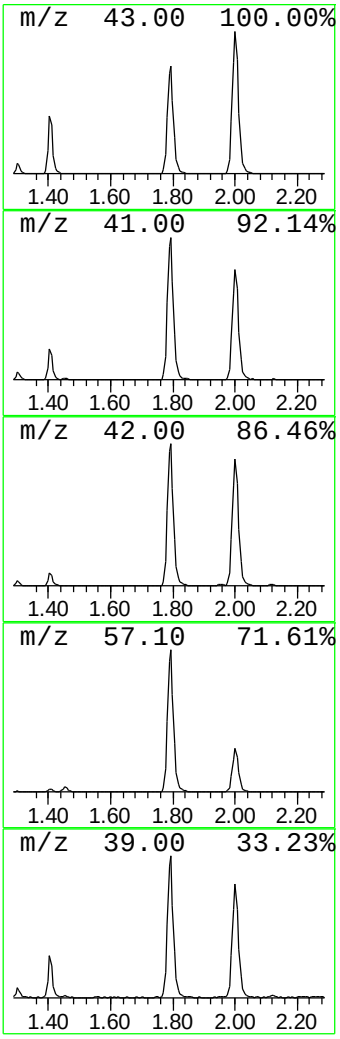
****

Peak Number 1 Butane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	91.04 ug/l	798762	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	33
3	3-Buten-1-ol	72	C4H8O	000627-27-0	25
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	16
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010963.D
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Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

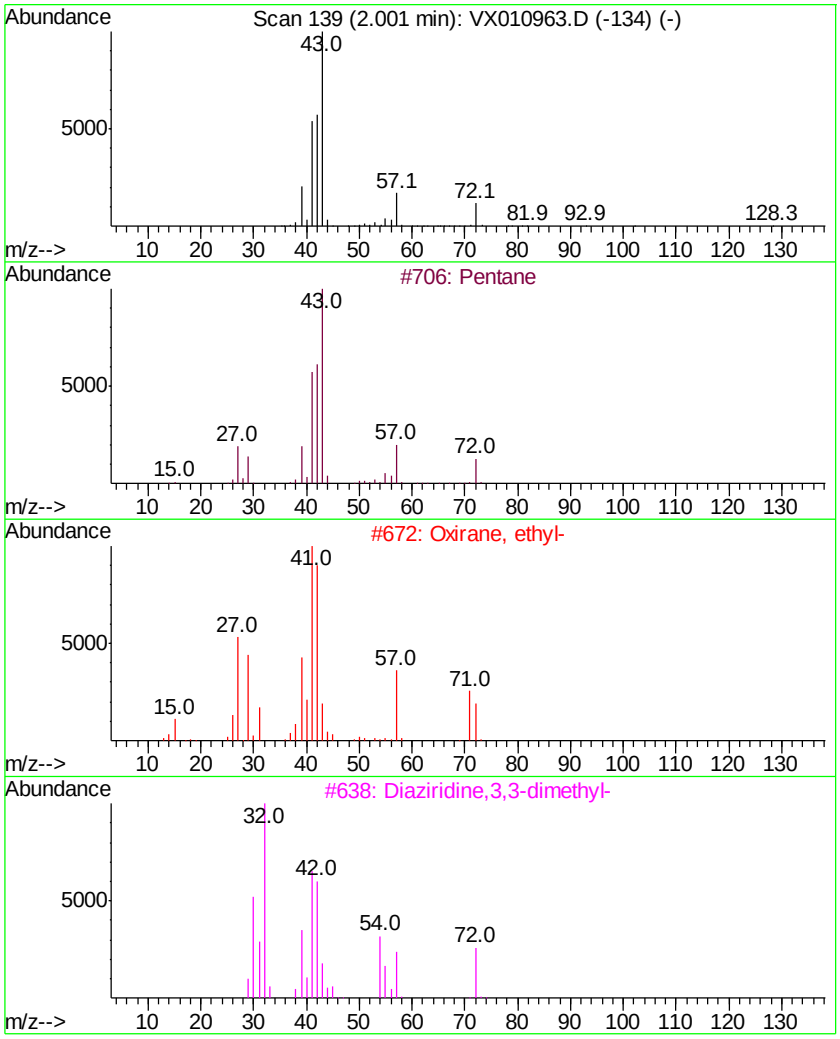
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

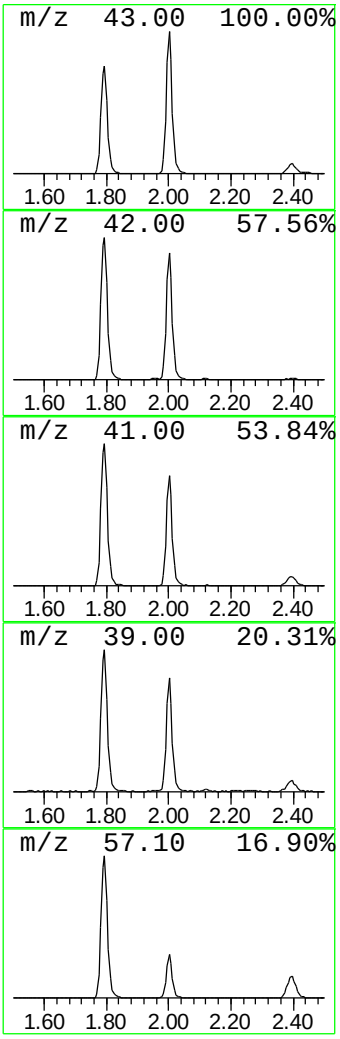
****

Peak Number 2 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	73.24 ug/l	642573	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	25
4	Butane, 2-methyl-	72	C5H12	000078-78-4	9
5	Isobutyl nitrite	103	C4H9NO2	000542-56-3	9





Library Search Compound Report

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Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

TIC Library : C:\DATABASE\NIST11.L
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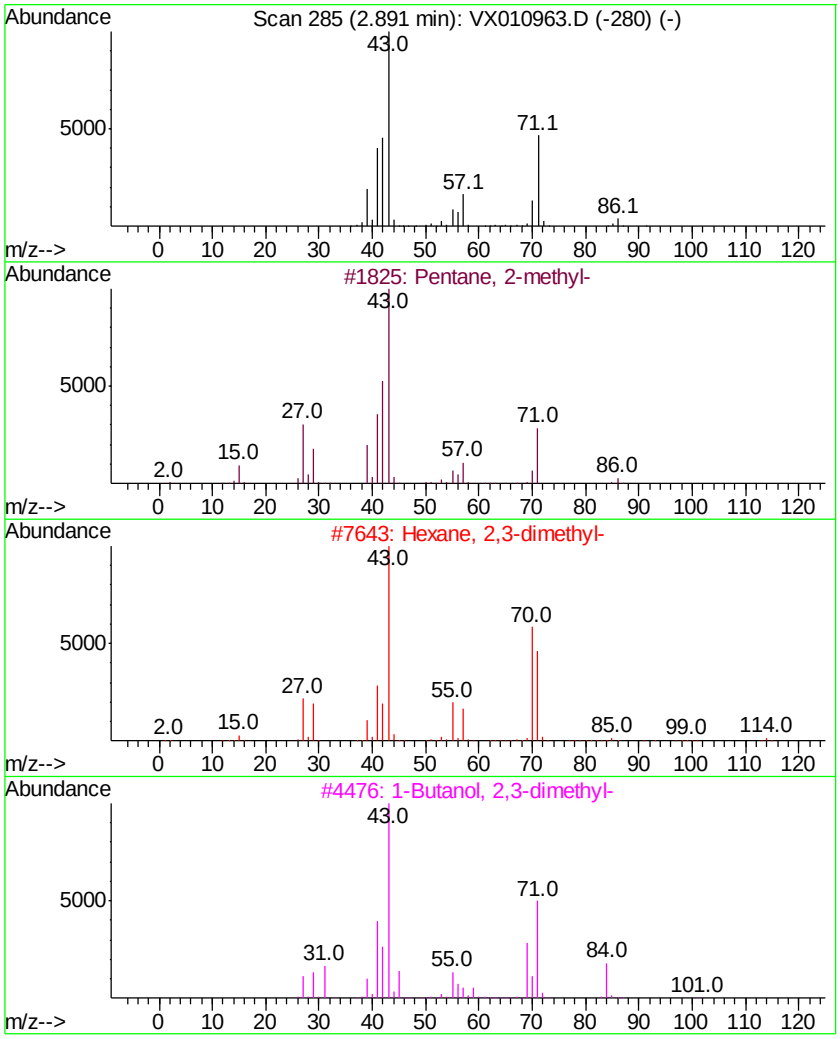
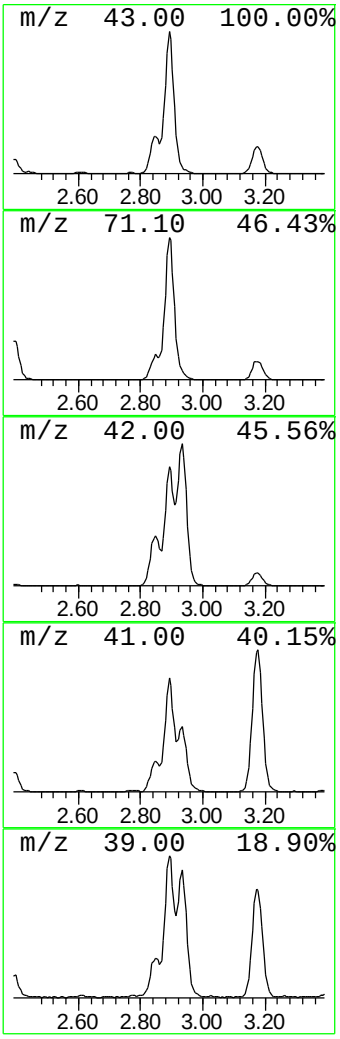
****

Peak Number 3 Pentane, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	82.69 ug/l	725522	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
2	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	47
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	72	C5H12	000109-66-0	38





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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

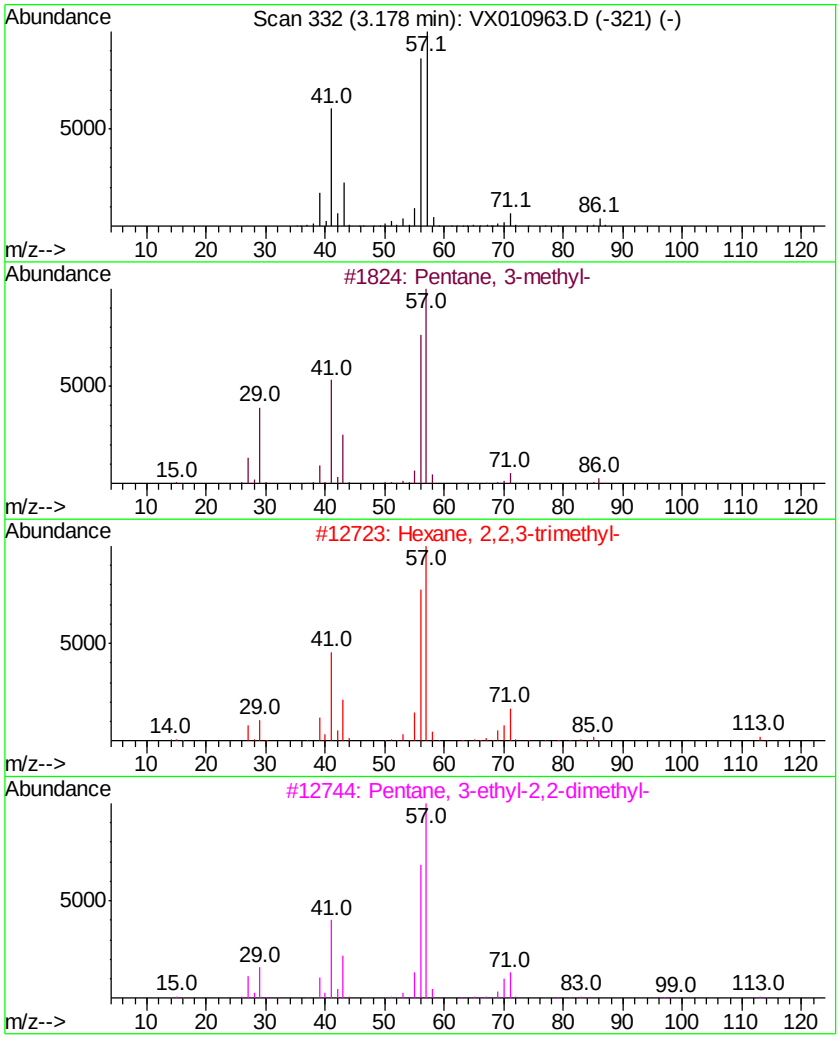
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

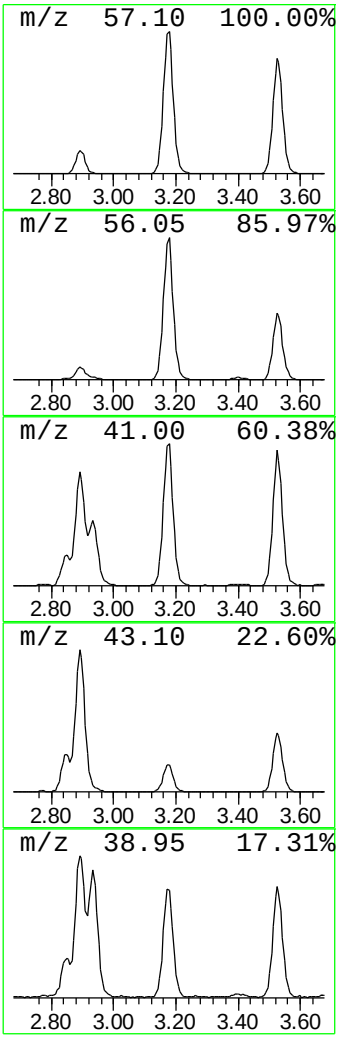
****

Peak Number 4 Pentane, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	80.04 ug/l	702241	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	64
4	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40
5	Sulphuric acid dibutyl ester	210	C8H18O4S	000625-22-9	40





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ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

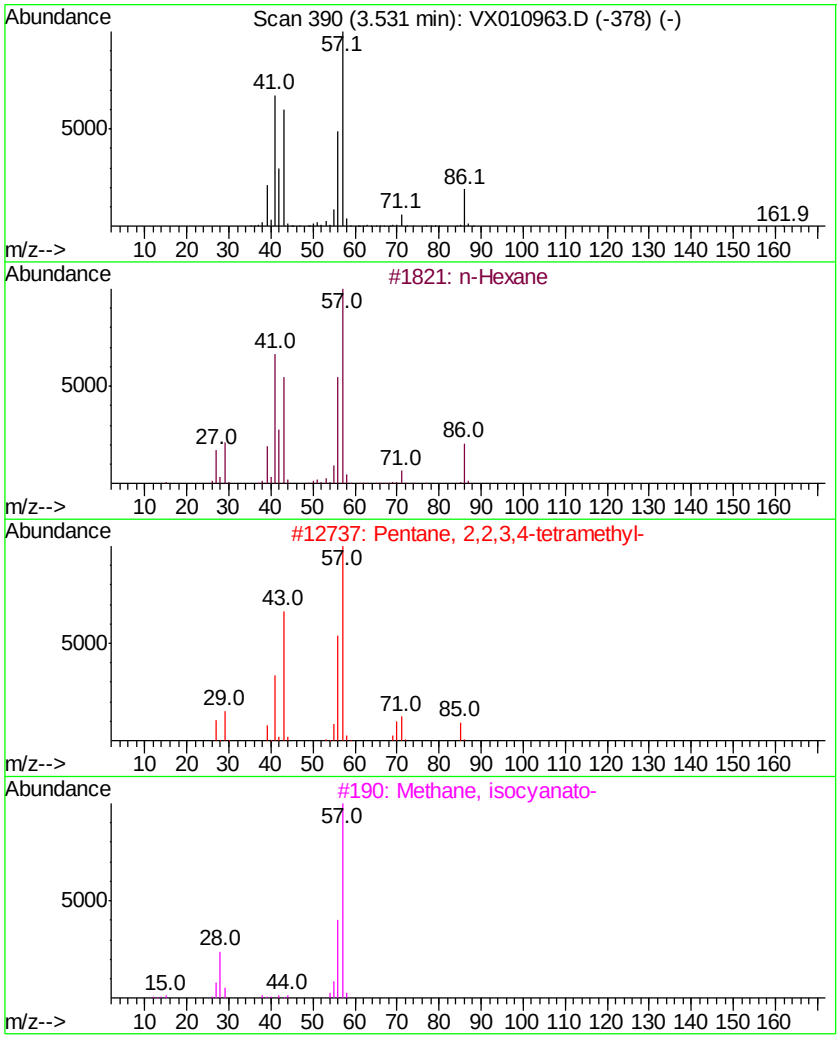
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

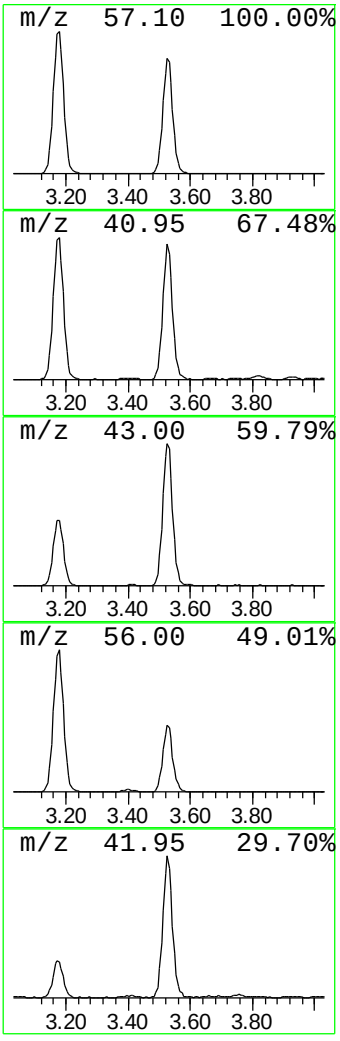
****

Peak Number 5 n-Hexane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	74.29 ug/l	651803	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexane	86	C6H14	000110-54-3	94
2	Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	42
3	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35
5	Butanal, 2-methyl-	86	C5H10O	000096-17-3	35





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Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

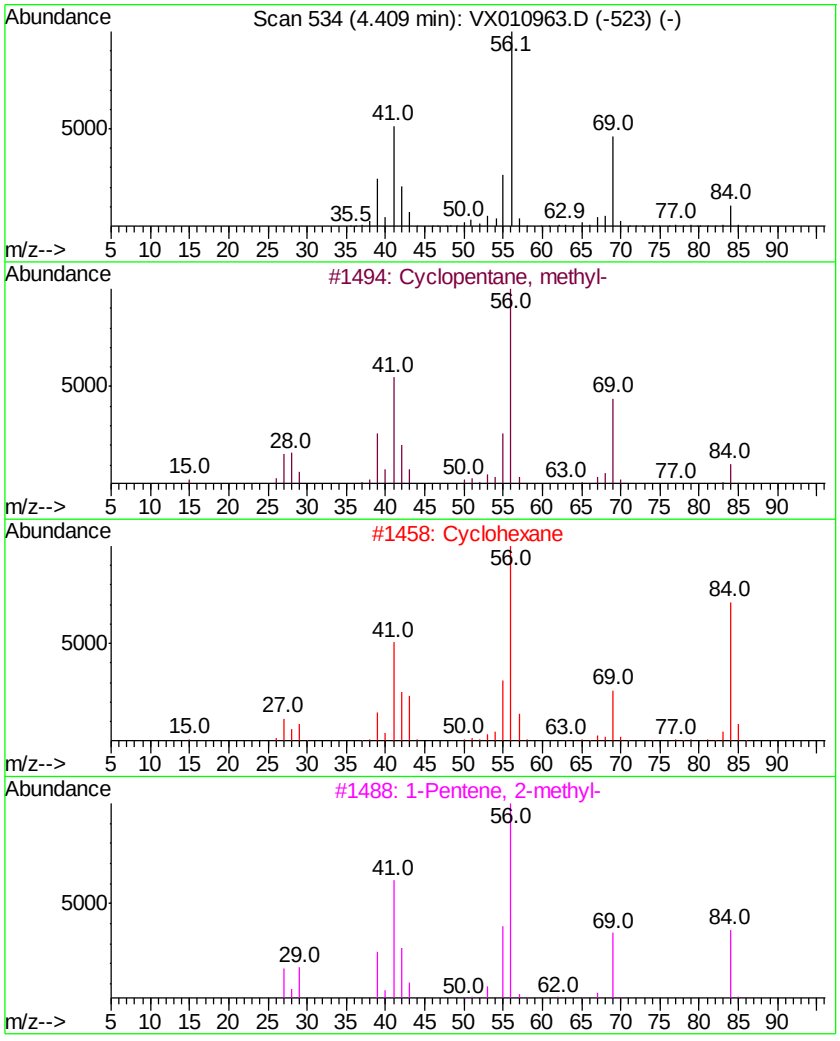
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

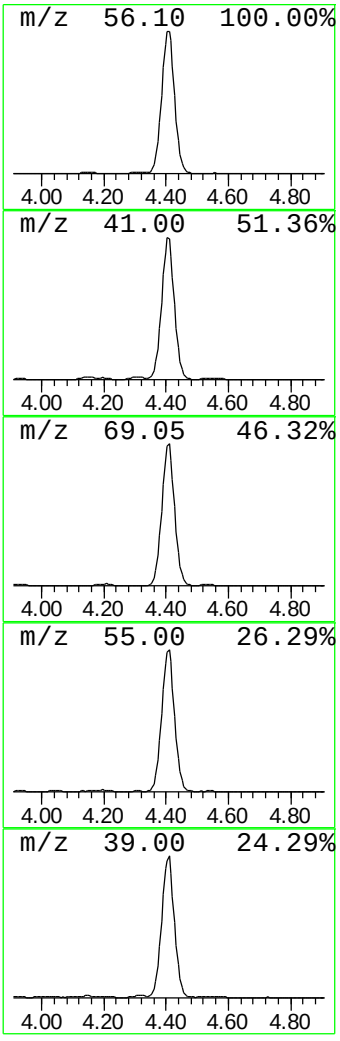
****

Peak Number 6 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	249.03 ug/l	2184900	Pentafluorobenzene	5.66

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	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72





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Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

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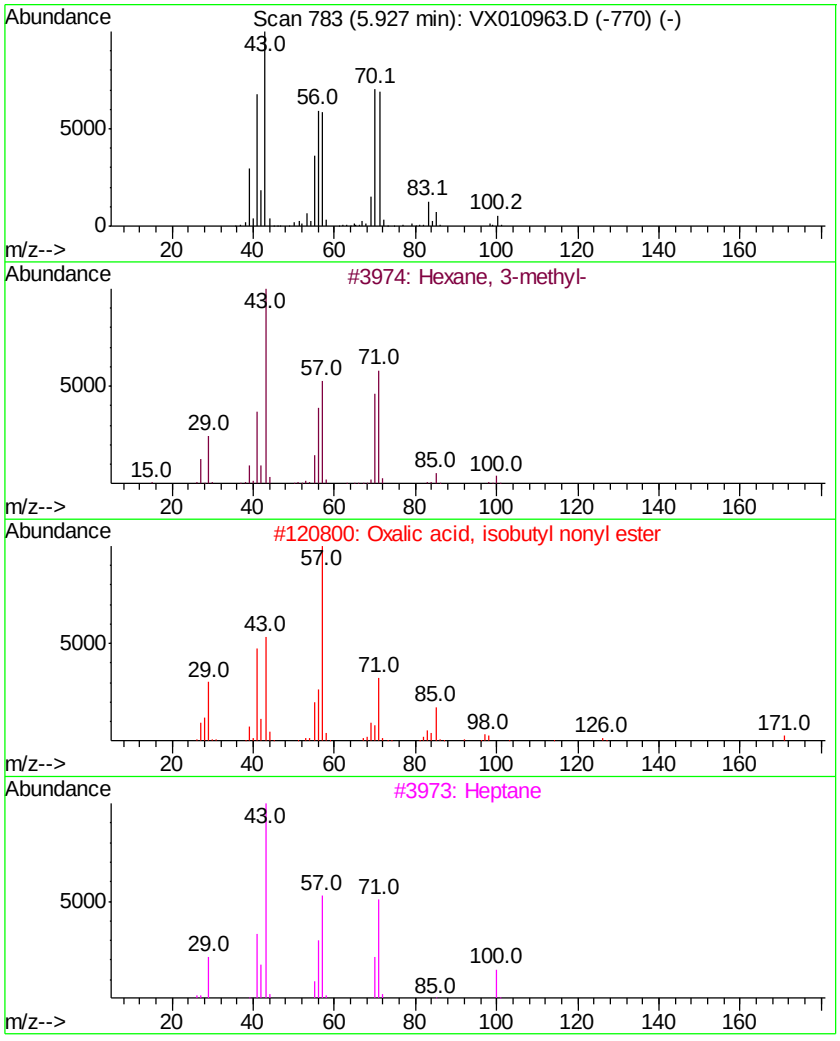
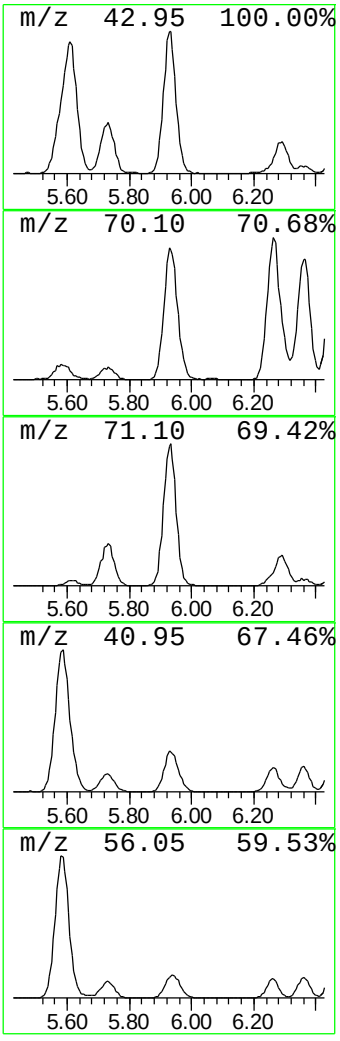
Peak Number 7 Hexane, 3-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	74.20 ug/l	651017	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	86
2	Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1000309-37-4	53
3	Heptane	100	C7H16	000142-82-5	50
4	Propanoic acid, 2-methyl-, 3-met...	158	C9H18O2	002050-01-3	50
5	Heptane, 4-methyl-	114	C8H18	000589-53-7	50





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

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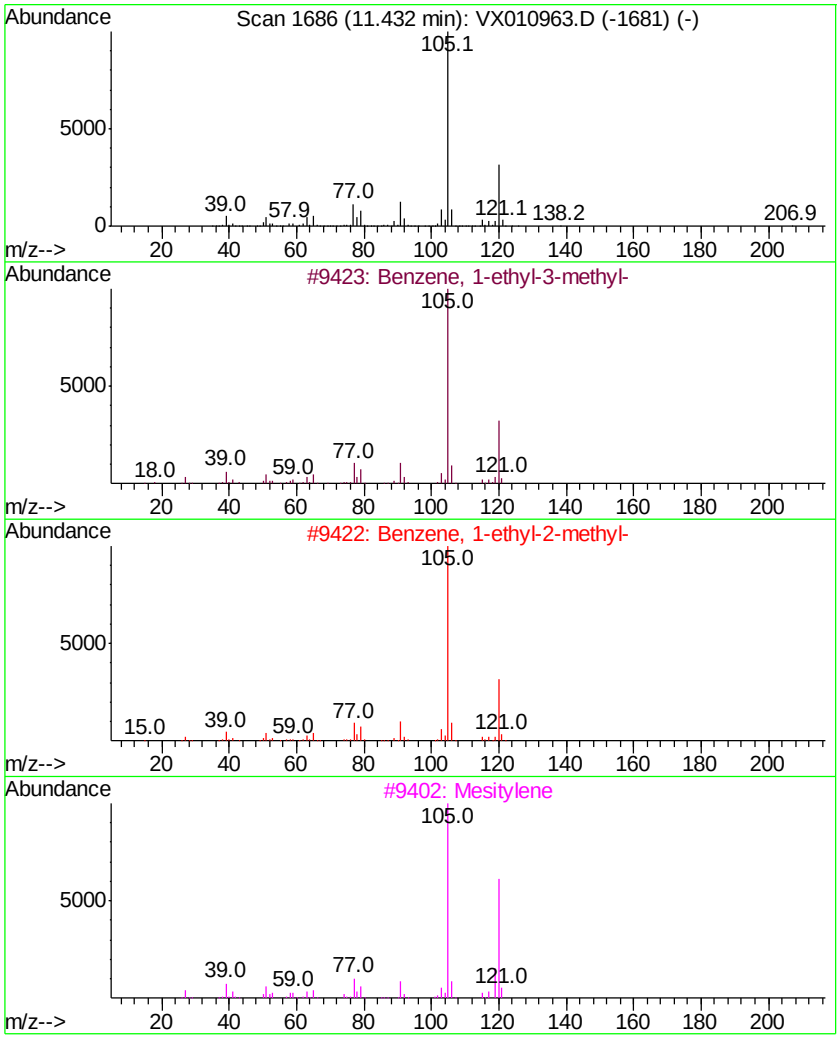
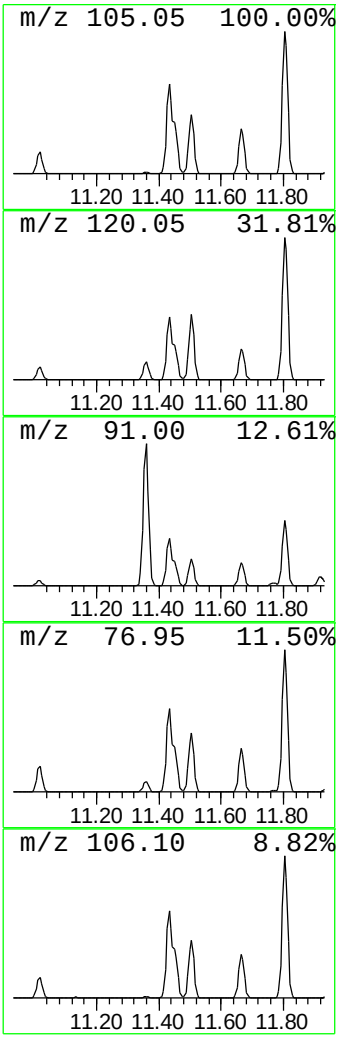
Peak Number 8 Benzene, 1-ethyl-3-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	172.52 ug/l	4188950	1,4-Dichlorobenzene-d4	12.08

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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

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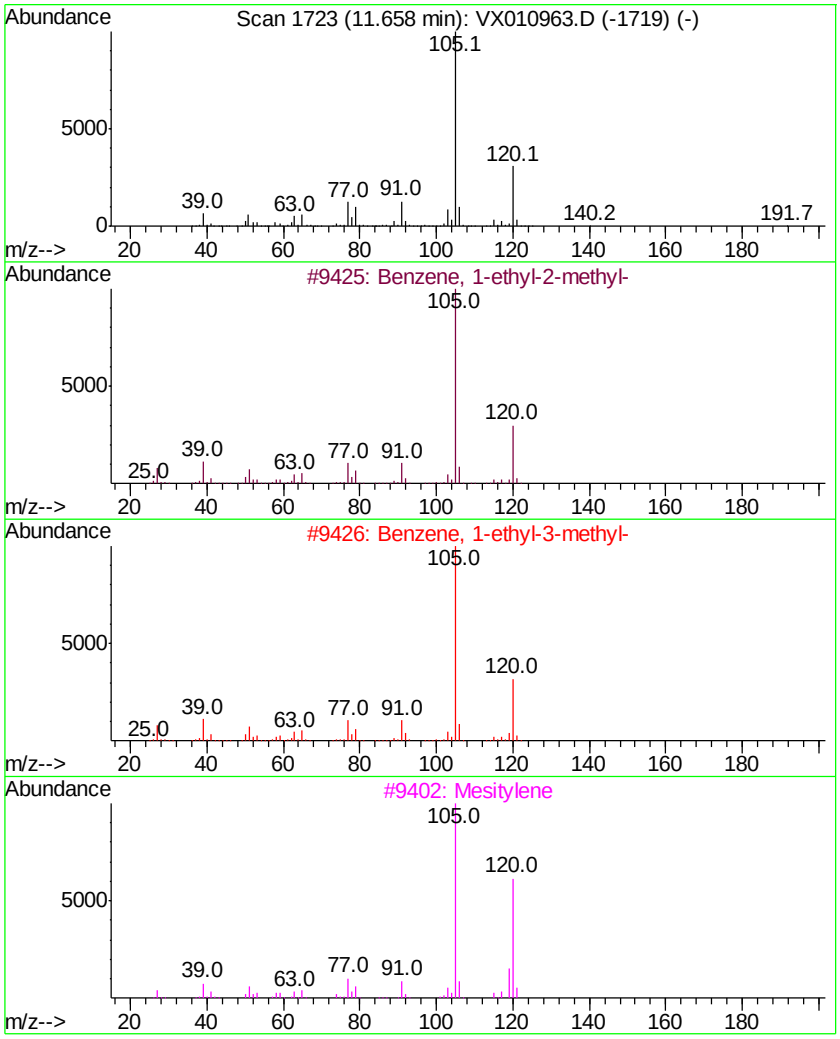
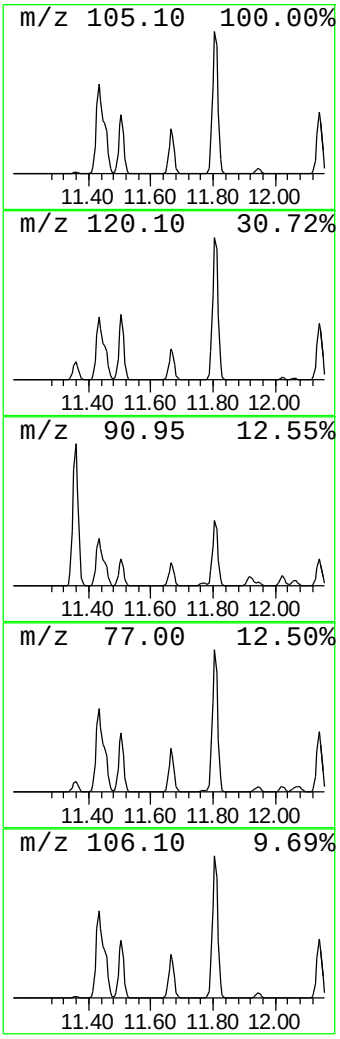
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.66	60.95 ug/l	1479820	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	94
2	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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

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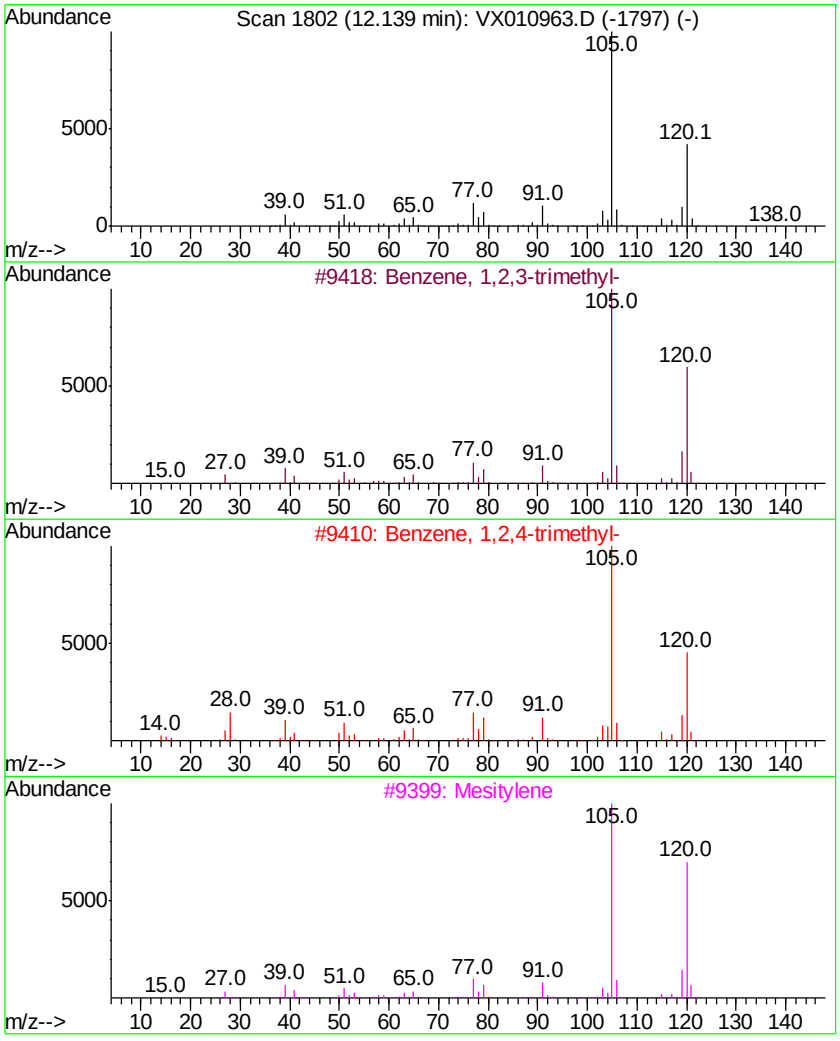
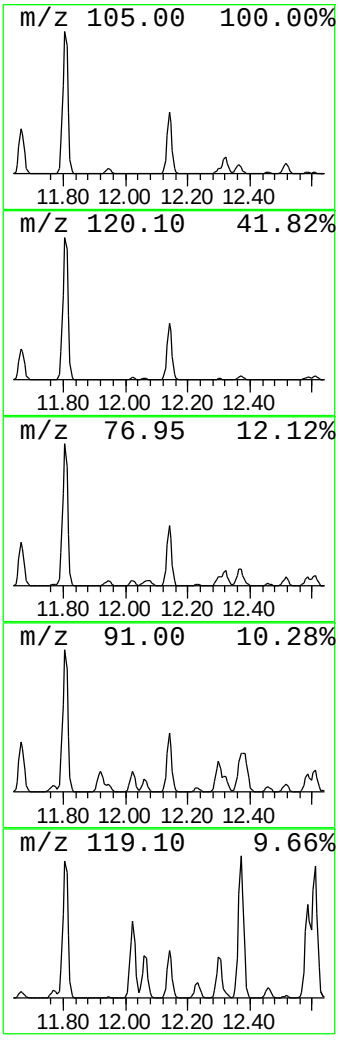
Peak Number 10 Benzene, 1,2,3-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	84.43 ug/l	2050010	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	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010963.D
Acq On : 18 Jul 2019 16:56
Operator : JC/SP
Sample : K3884-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0612

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	91.0	ug/l	798762	1	5.66	438679	50.0
Pentane	2.00	73.2	ug/l	642573	1	5.66	438679	50.0
Pentane, 2-methyl-	2.89	82.7	ug/l	725522	1	5.66	438679	50.0
Pentane, 3-methyl-	3.18	80.0	ug/l	702241	1	5.66	438679	50.0
n-Hexane	3.53	74.3	ug/l	651803	1	5.66	438679	50.0
Cyclopentane, met...	4.41	249.0	ug/l	2184900	1	5.66	438679	50.0
Hexane, 3-methyl-	5.93	74.2	ug/l	651017	1	5.66	438679	50.0
Benzene, 1-ethyl-...	11.43	172.5	ug/l	4188950	4	12.08	1214050	50.0
Benzene, 1-ethyl-...	11.66	61.0	ug/l	1479820	4	12.08	1214050	50.0
Benzene, 1,2,3-tr...	12.14	84.4	ug/l	2050010	4	12.08	1214050	50.0