LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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	1.788	99	104	116	rVB	931874	1360131	3.01%	0.669%
2	2.001	133	139	155	rVB	1104154	1561395	3.46%	0.768%
3	2.849	270	278	280	rBV	344083	699560	1.55%	0.344%
4	2.891	280	285	313	rVB	1421062	3417979	7.57%	1.681%
5	3.178	320	332	349	rBV	1235827	2878042	6.38%	1.415%
6	3.525	379	389	405	rBV	1354640	3105064	6.88%	1.527%
7	4.409	523	534	547	rVB	2271644	6693797	14.83%	3.292%
8	5.586	717	727	737	rBV2	1628716	5282058	11.71%	2.598%
9	5.726	745	750	772	rVB	181475	571177	1.27%	0.281%
10	5.933	772	784	797	rBV3	473179	1530042	3.39%	0.752%
11	6.263	822	838	847	rBV2	222236	751764	1.67%	0.370%
12	6.360	847	854	862	rVV	216594	591411	1.31%	0.291%
13	6.458	862	870	881	rVB	343871	940163	2.08%	0.462%
14	6.708	900	911	920	rBV2	283684	688718	1.53%	0.339%
15	6.860	927	936	943	rBV	363819	863609	1.91%	0.425%
16	7.464	1021	1035	1047	rBV	2311128	5285681	11.71%	2.599%
17	8.713	1235	1240	1248	rVB	822542	1361107	3.02%	0.669%
18	10.109	1464	1469	1475	rVB	764017	1036877	2.30%	0.510%
19	10.256	1486	1493	1498	rBV	12148926	16503767	36.57%	8.116%
20	10.365	1502	1511	1517	rBV	29317882	45125451	100.00%	22.192%
21	10.701	1560	1566	1572	rVB	16703687	21923041	48.58%	10.781%
22	11.018	1612	1618	1631	rVB	1316848	1659146	3.68%	0.816%
23	11.134	1631	1637	1642	rBV	744404	941374	2.09%	0.463%
24	11.359	1665	1674	1681	rBV	1994945	2380091	5.27%	1.170%
25	11.432	1681	1686	1694	rVV	6825627	12338475	27.34%	6.068%
26	11.506	1694	1698	1705	rVB	4753889	5588692	12.38%	2.748%
27	11.664	1719	1724	1733	rBV	3726131	4651223	10.31%	2.287%
28	11.810	1742	1748	1753	rVB	11554980	14259953	31.60%	7.013%
29	12.024	1777	1783	1786	rBV	465153	552699	1.22%	0.272%
30	12.072	1786	1791	1797	rVB2	984019	1463554	3.24%	0.720%
31	12.140	1797	1802	1808	rBV	5651943	7016261	15.55%	3.450%
32	12.298	1822	1828	1835	rBV2	3070984	4564166	10.11%	2.245%
33	12.371	1835	1840	1849	rVB3	1327192	1950810	4.32%	0.959%
34	12.518	1859	1864	1870	rBV	455045	544265	1.21%	0.268%

LSC Area Percent Report

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Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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	12.585	1870	1875	1877	rBV	717616	929201	2.06%	0.457%
36	12.609	1877	1879	1883	rVV	820767	823318	1.82%	0.405%
37	12.664	1883	1888	1892	rVV	963195	1239032	2.75%	0.609%
38	12.755	1898	1903	1911	rVV3	678421	1161496	2.57%	0.571%
39	12.902	1922	1927	1932	rVB2	550504	707087	1.57%	0.348%
40	12.975	1932	1939	1942	rVV	793759	962982	2.13%	0.474%
41	13.017	1942	1946	1952	rVB	1192636	1430053	3.17%	0.703%
42	13.225	1976	1980	1984	rVB	535684	638162	1.41%	0.314%
43	13.347	1995	2000	2005	rVB2	1875714	2670391	5.92%	1.313%
44	13.475	2016	2021	2028	rVB	956007	1231243	2.73%	0.606%
45	13.834	2071	2080	2088	rBV	5974144	7360698	16.31%	3.620%
46	14.694	2213	2221	2226	rBV	2046582	2453761	5.44%	1.207%
47	14.834	2239	2244	2253	rBV	1283949	1653880	3.67%	0.813%

Sum of corrected areas: 203342847

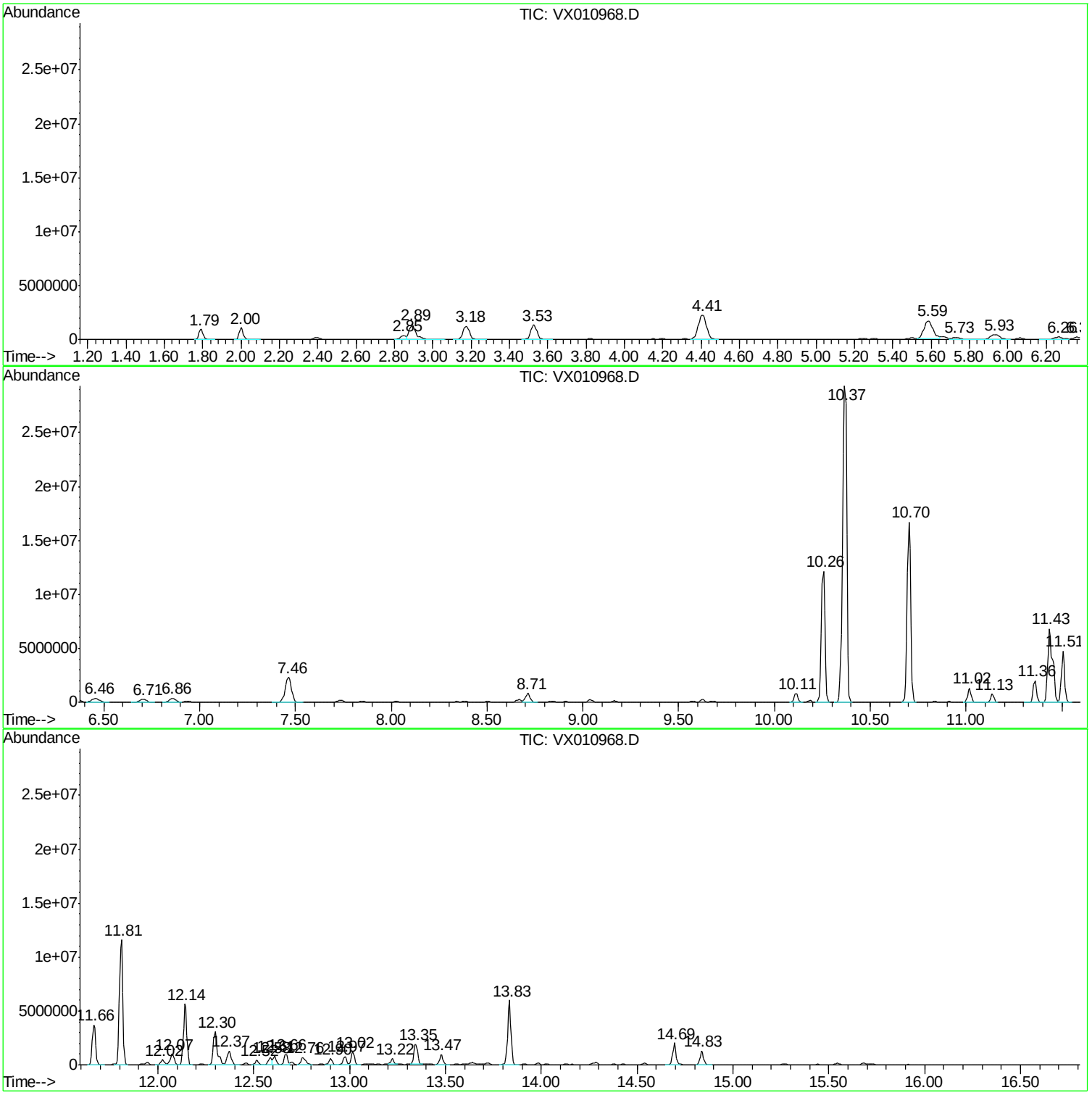
LSC Report - Integrated Chromatogram

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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 : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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

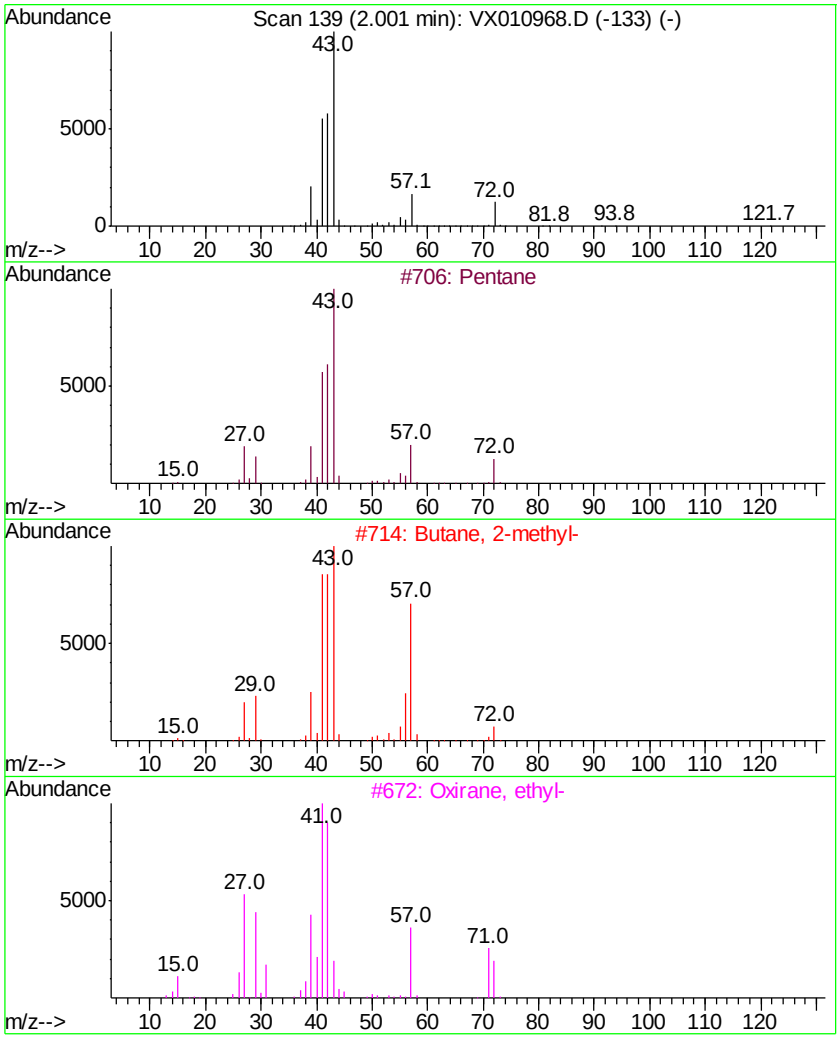
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

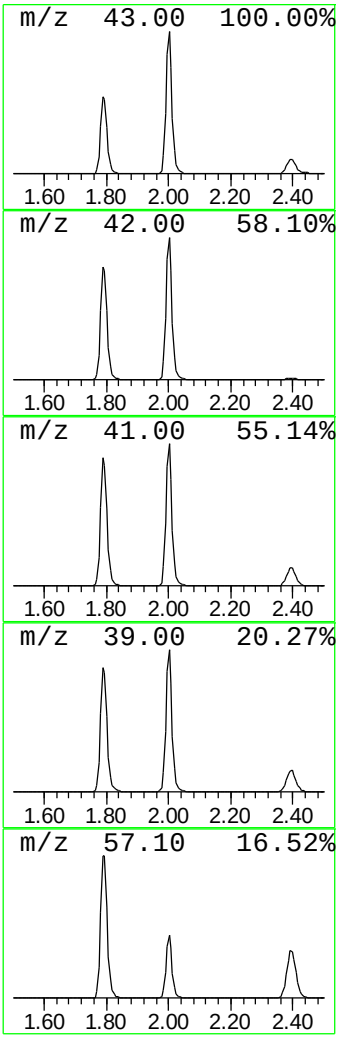
****

Peak Number 1 Pentane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	136.68 ug/l	1561400	Pentafluorobenzene	5.66

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	Cyclobutylamine	71	C4H9N	002516-34-9	9





Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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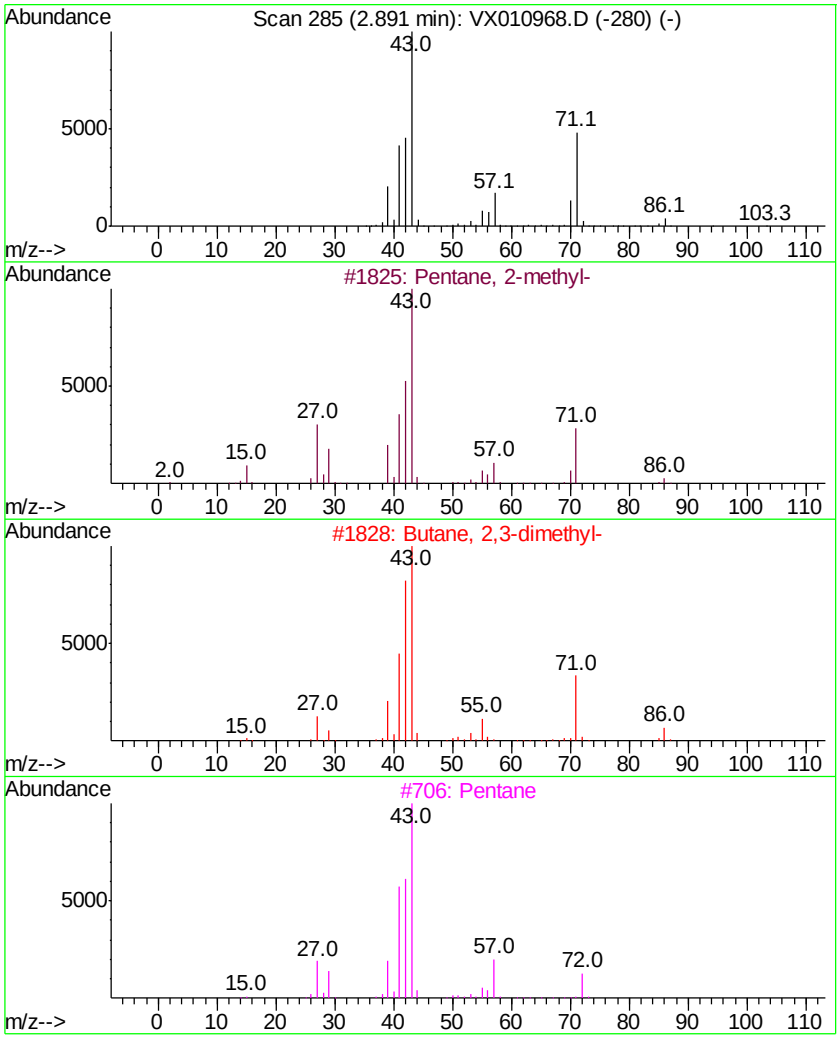
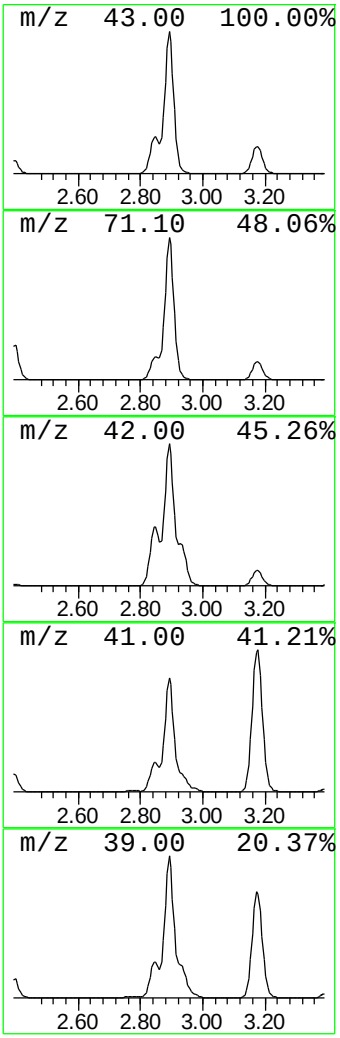
Peak Number 2 Pentane, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	299.21 ug/l	3417980	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	64
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3	Pentane	72	C5H12	000109-66-0	46
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	45
5	Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	38





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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

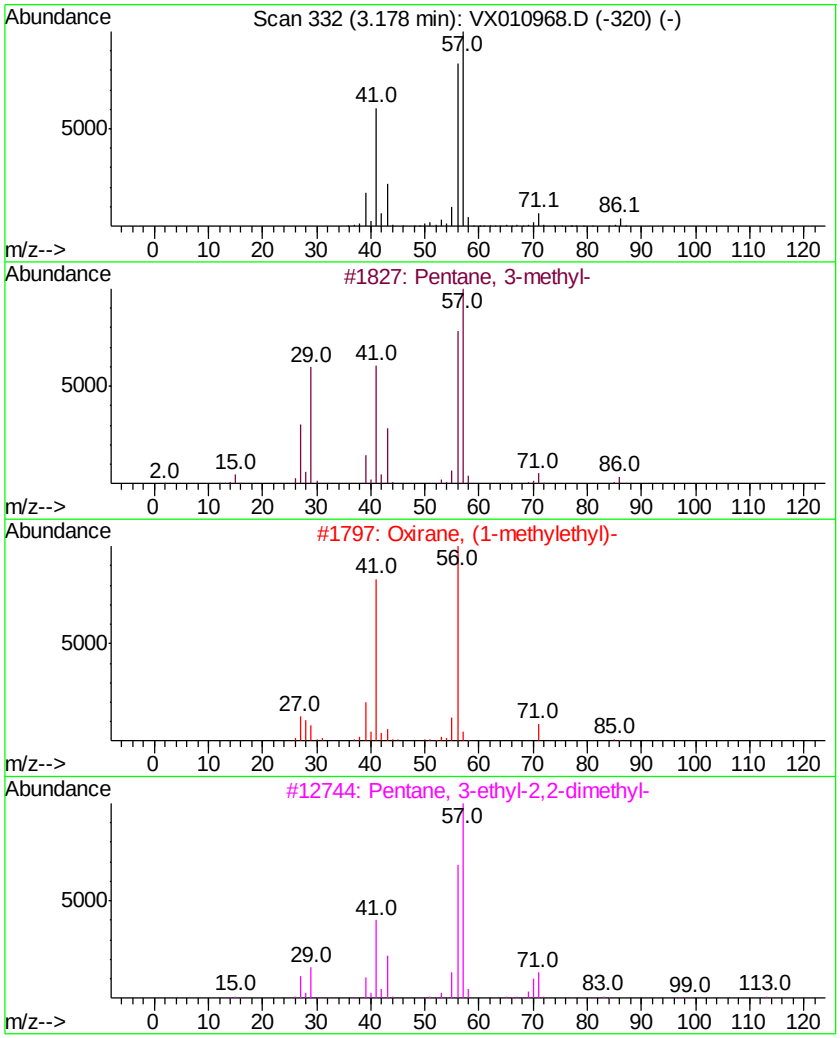
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

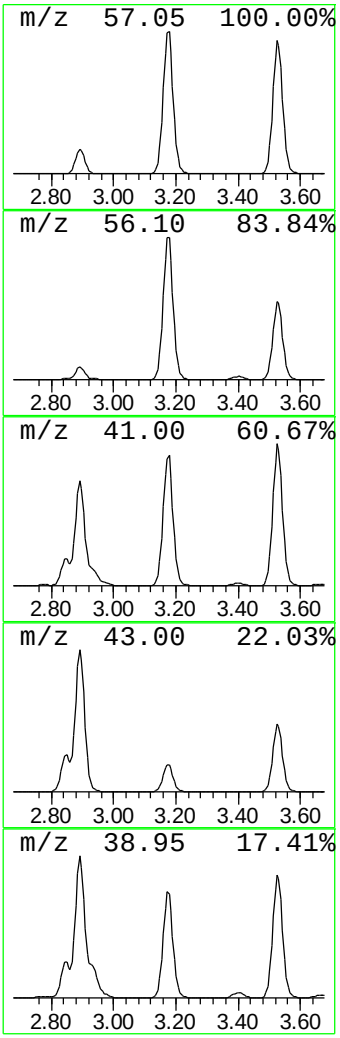
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.18	251.94 ug/l	2878040	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	91
2	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	43
5	Butyl isocyanatoacetate	157	C7H11NO3	017046-22-9	40





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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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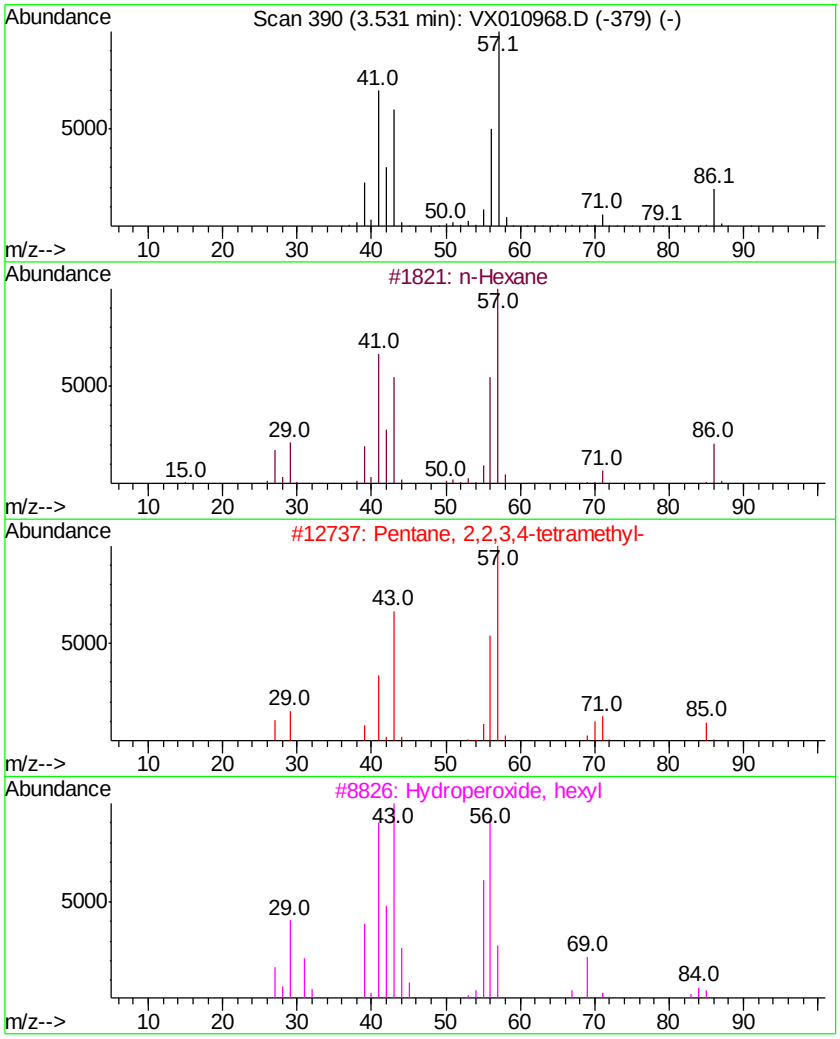
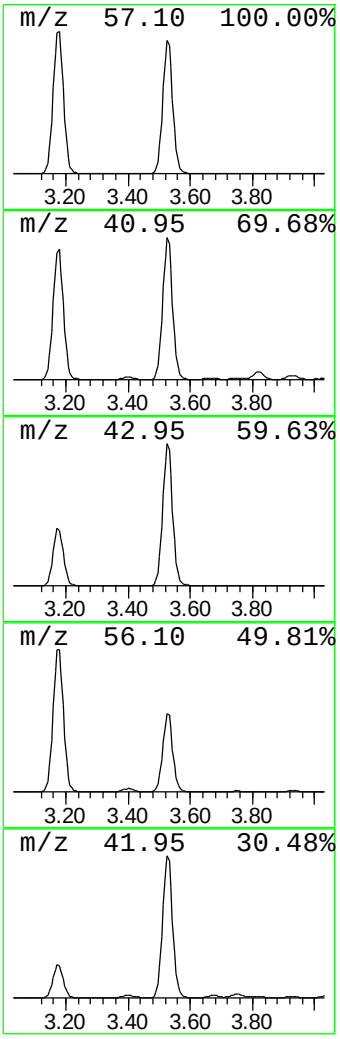
Peak Number 4 n-Hexane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	271.81 ug/l	3105060	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	53
3	Hydroperoxide, hexyl	118	C6H14O2	004312-76-9	40
4	Methane, isocyanato-	57	C2H3NO	000624-83-9	37
5	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	35





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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

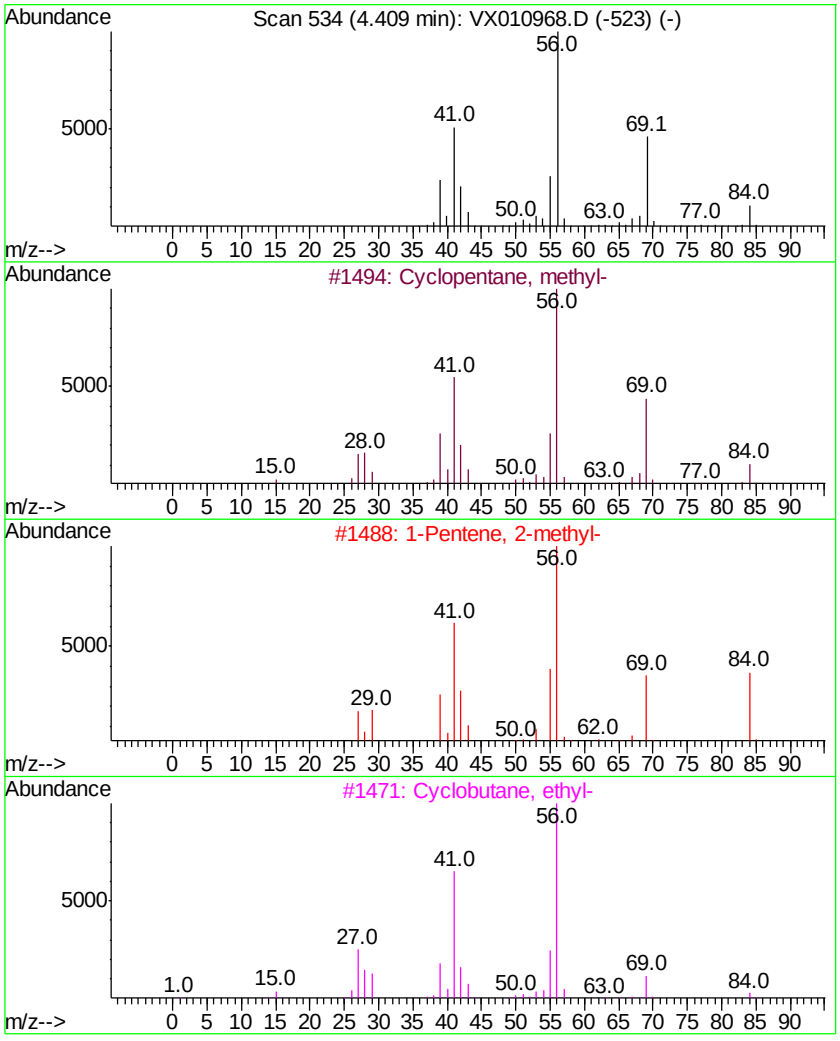
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

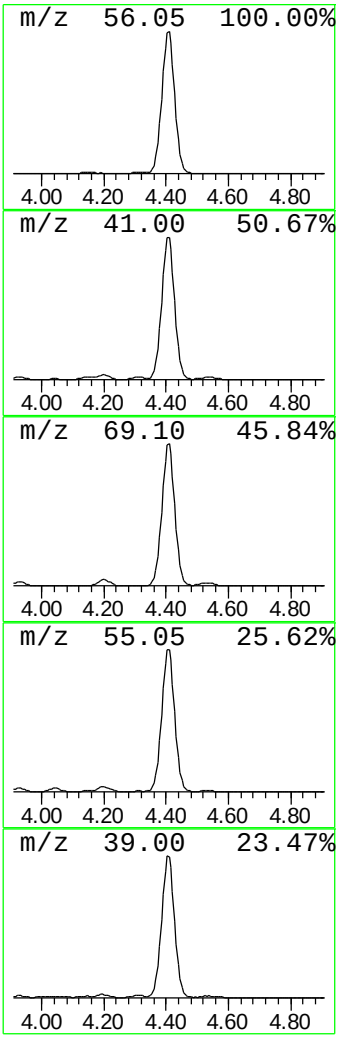
****

Peak Number 5 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.41	585.97 ug/l	6693800	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	Cyclohexane	84	C6H12	000110-82-7	56





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Operator : JC/SP
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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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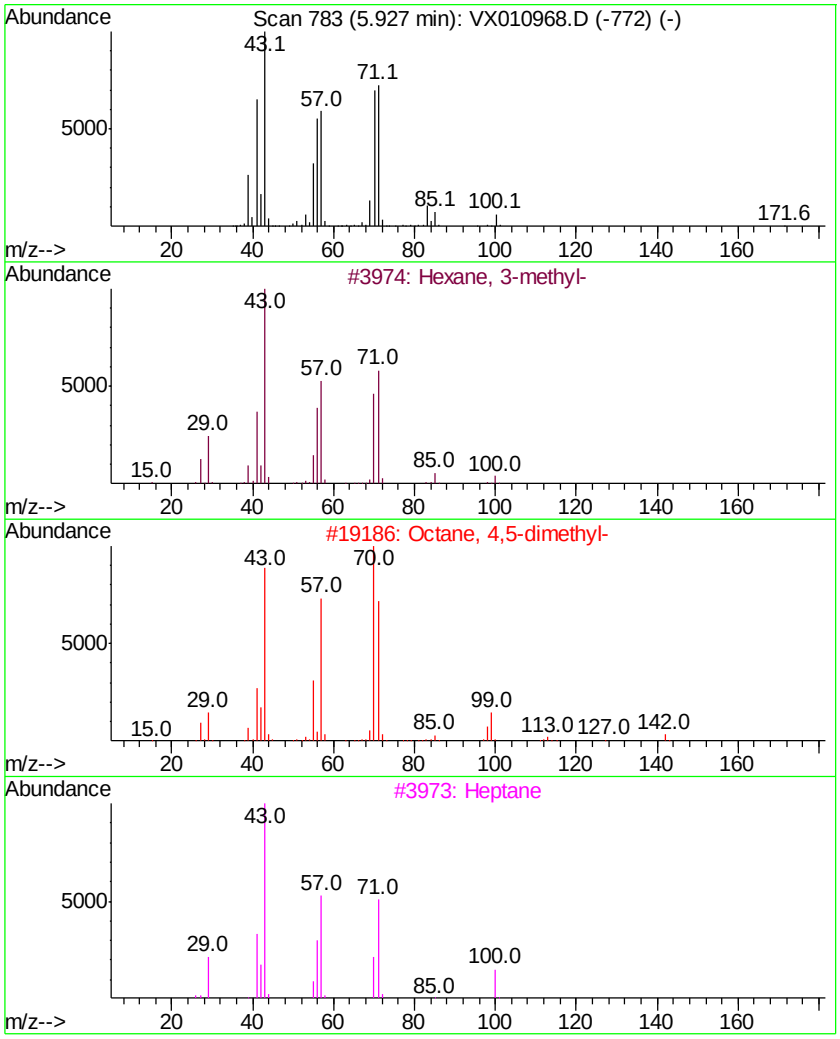
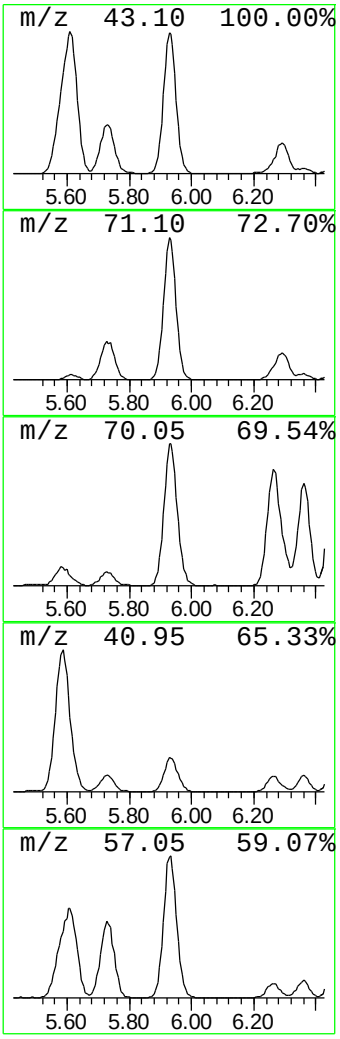
Peak Number 6 Hexane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	133.94 ug/l	1530040	Pentafluorobenzene	5.66

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexane, 3-methyl-	100	C7H16	000589-34-4	86
2	Octane, 4,5-dimethyl-	142	C10H22	015869-96-2	53
3	Heptane	100	C7H16	000142-82-5	50
4	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	47
5	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	47





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Instrument : MSVOA_X
ClientSampleId : FL-0616

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

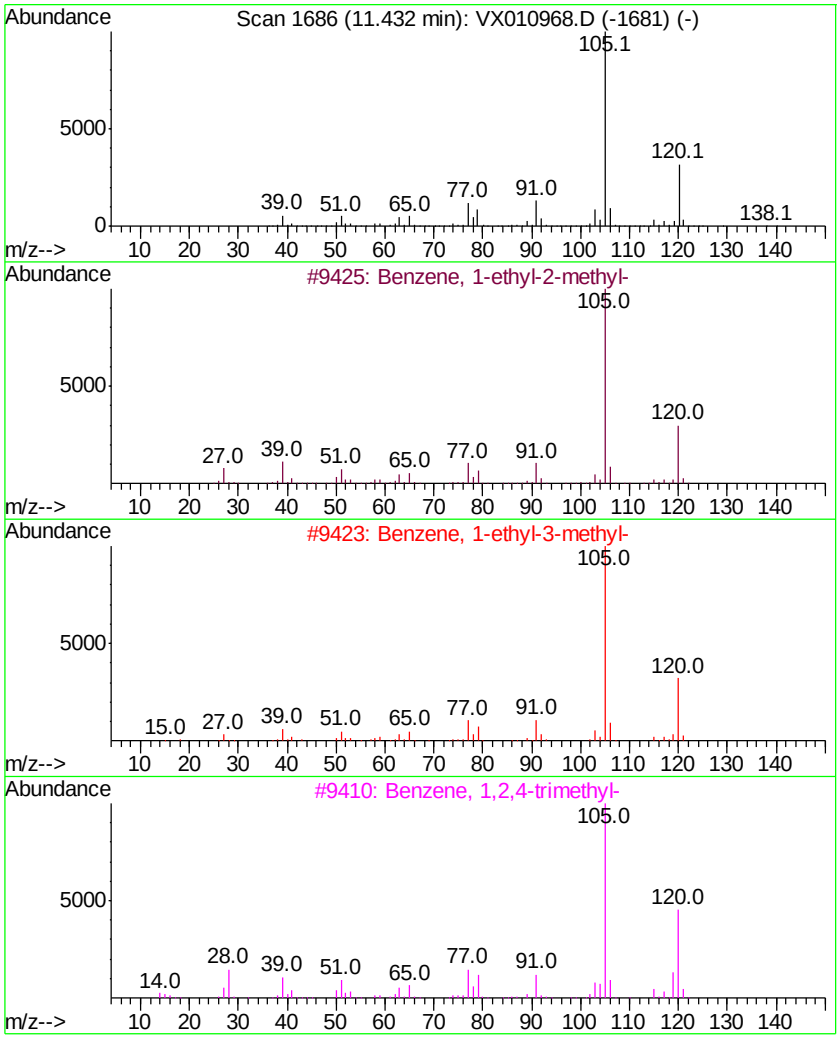
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

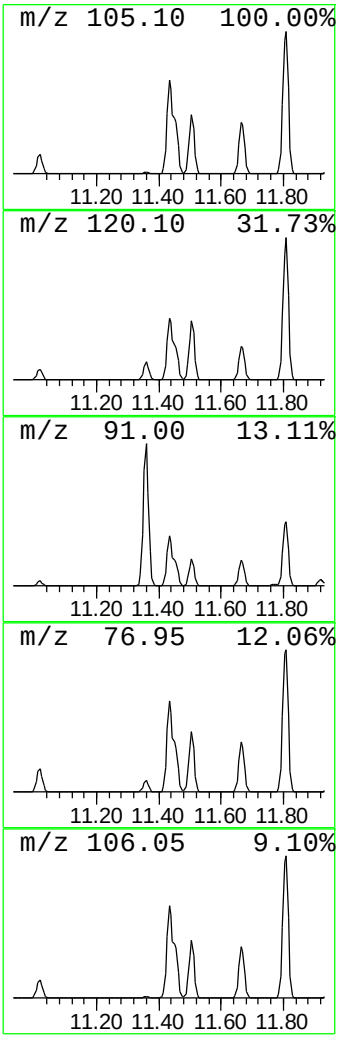
****

Peak Number 7 Benzene, 1-ethyl-2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.43	421.52 ug/l	12338500	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, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
5	Mesitylene	120	C9H12	000108-67-8	91





Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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

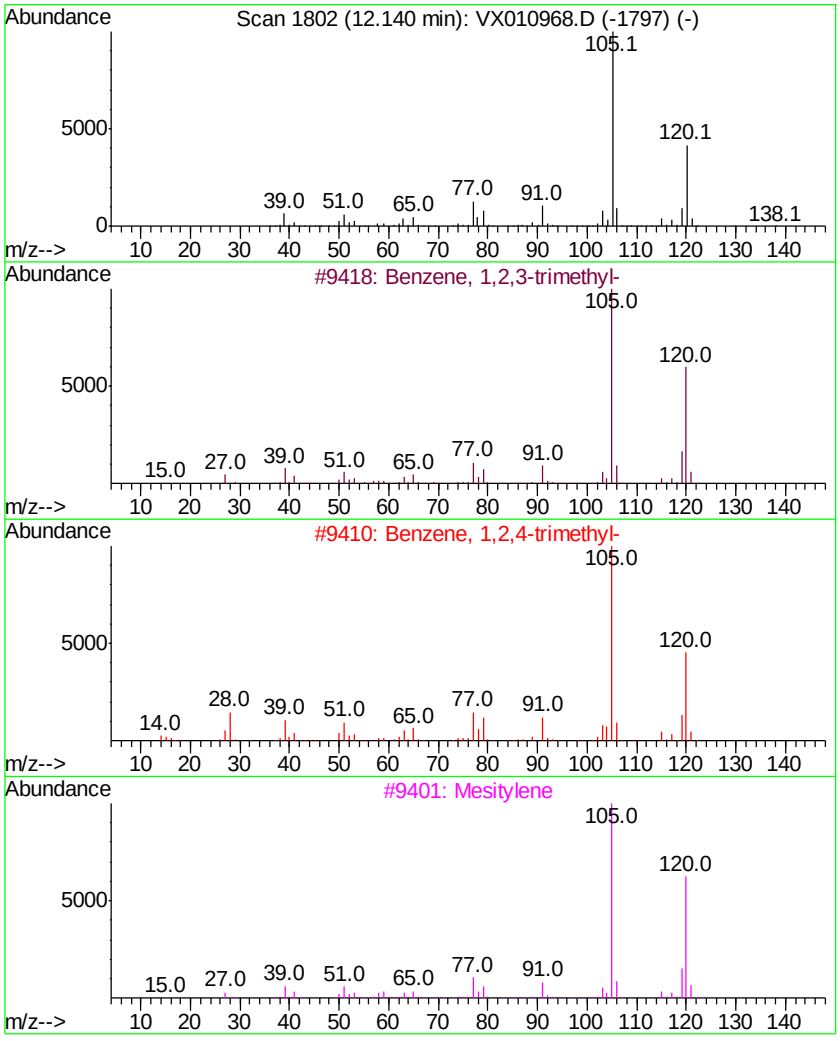
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

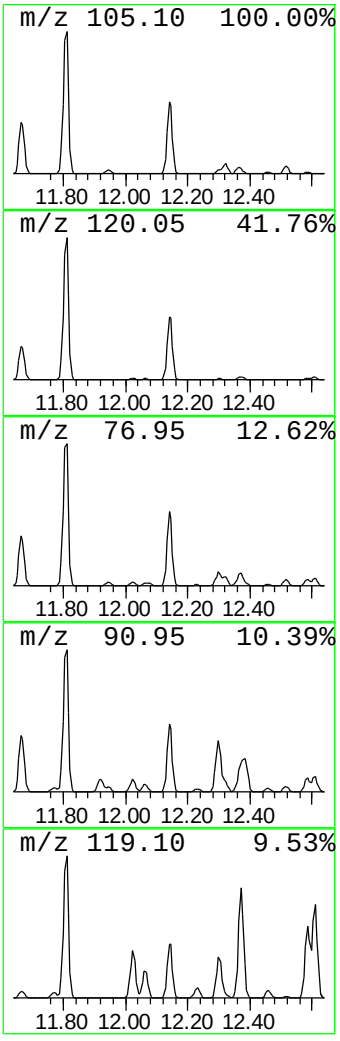
****

Peak Number 9 Benzene, 1,2,3-trimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.14	239.70 ug/l	7016260	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





Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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

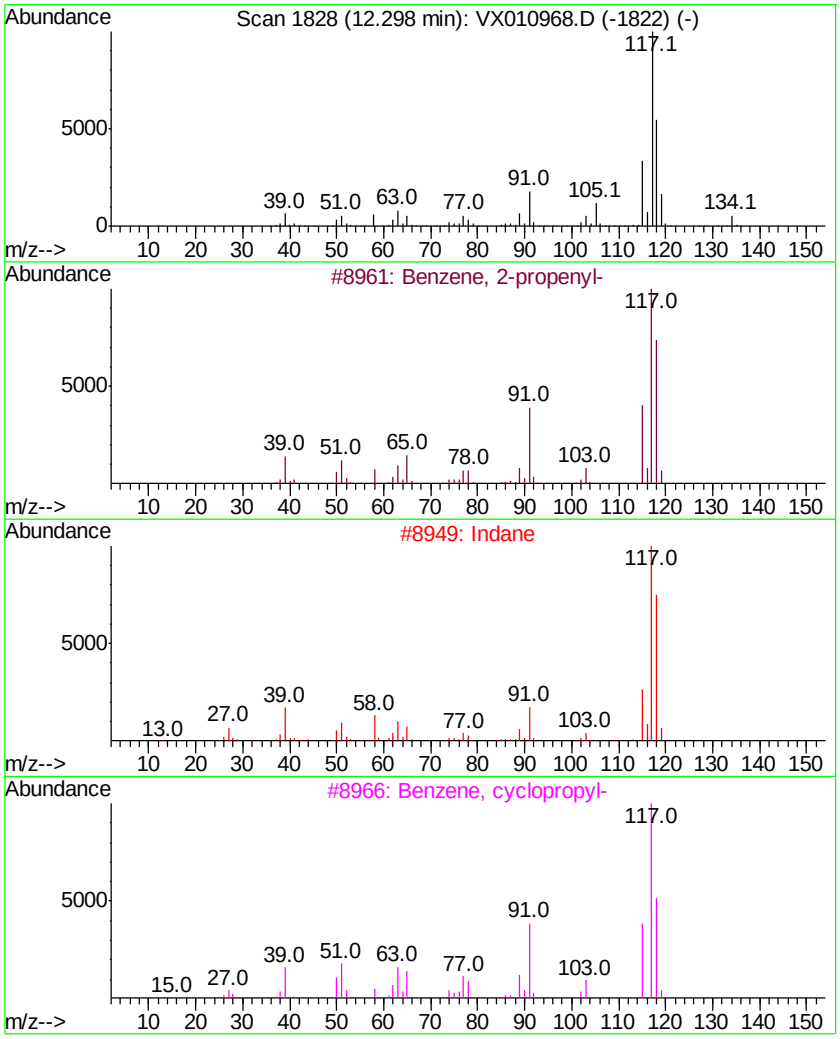
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

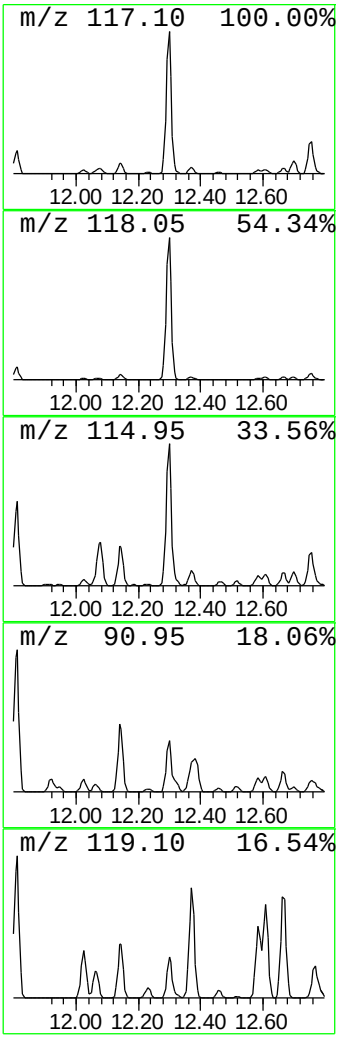
****

Peak Number 10 Benzene, 2-propenyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	155.93 ug/l	4564170	1,4-Dichlorobenzene-d4	12.08

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-propenyl-	118	C9H10	000300-57-2	76
2	Indane	118	C9H10	000496-11-7	76
3	Benzene, cyclopropyl-	118	C9H10	000873-49-4	76
4	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	59
5	Deltacyclene	118	C9H10	007785-10-6	58





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_X\DATA\VX071819\
Data File : VX010968.D
Acq On : 18 Jul 2019 18:52
Operator : JC/SP
Sample : K3884-08
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 23 Sample Multiplier: 1

Instrument : MSVOA_X
ClientSampleId : FL-0616

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
Pentane	2.00	136.7	ug/l	1561400	1	5.66	571177	50.0
Pentane, 2-methyl-	2.89	299.2	ug/l	3417980	1	5.66	571177	50.0
Pentane, 3-methyl-	3.18	251.9	ug/l	2878040	1	5.66	571177	50.0
n-Hexane	3.53	271.8	ug/l	3105060	1	5.66	571177	50.0
Cyclopentane, met...	4.41	586.0	ug/l	6693800	1	5.66	571177	50.0
Hexane, 3-methyl-	5.93	133.9	ug/l	1530040	1	5.66	571177	50.0
Benzene, 1-ethyl-...	11.43	421.5	ug/l	12338500	4	12.08	1463550	50.0
Benzene, 1,2,3-tr...	12.14	239.7	ug/l	7016260	4	12.08	1463550	50.0
Benzene, 2-propenyl-	12.30	155.9	ug/l	4564170	4	12.08	1463550	50.0