LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
Sample : J2132-05 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.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	1.075	76	80	92	rBV	321617	386354	19.52%	3.373%
2	1.404	130	134	140	rBV	87095	87214	4.41%	0.761%
3	1.794	192	198	209	rBV	281715	388631	19.64%	3.393%
4	1.953	220	224	228	rBV	24274	33524	1.69%	0.293%
5	2.001	228	232	245	rVB2	126300	237249	11.99%	2.071%
6	2.123	245	252	258	rBV	71923	107817	5.45%	0.941%
7	2.221	262	268	272	rBV	42178	61243	3.09%	0.535%
8	2.270	272	276	283	rVB	118814	184651	9.33%	1.612%
9	2.818	353	366	370	rBV2	18775	60779	3.07%	0.531%
10	2.892	374	378	382	rVV2	43462	98418	4.97%	0.859%
11	2.934	382	385	398	rVB2	64078	139447	7.05%	1.217%
12	3.172	416	424	434	rBV2	30037	70304	3.55%	0.614%
13	3.404	453	462	471	rBV4	12748	35035	1.77%	0.306%
14	3.526	475	482	492	rVB3	19981	47353	2.39%	0.413%
15	3.818	524	530	539	rVB3	12797	31805	1.61%	0.278%
16	3.922	539	547	554	rBV5	7725	20968	1.06%	0.183%
17	4.202	583	593	599	rBV2	10905	28305	1.43%	0.247%
18	4.403	617	626	637	rVB3	39275	118068	5.97%	1.031%
19	5.312	765	775	787	rVB2	19133	56289	2.84%	0.491%
20	5.519	797	809	815	rBV	71312	207769	10.50%	1.814%
21	5.580	816	819	826	rVV3	21753	59643	3.01%	0.521%
22	5.678	826	835	848	rVB	116621	330116	16.68%	2.882%
23	6.080	890	901	910	rBV2	81130	207140	10.47%	1.808%
24	6.318	922	940	944	rBV7	8233	32382	1.64%	0.283%
25	6.872	1022	1031	1040	rBV	183786	438322	22.15%	3.826%
26	7.464	1117	1128	1138	rVB4	16824	41582	2.10%	0.363%
27	8.726	1328	1335	1340	rBV	389166	616039	31.13%	5.378%
28	8.793	1340	1346	1359	rVB	316032	480690	24.29%	4.196%
29	10.122	1556	1564	1573	rBV	427715	582041	29.41%	5.081%
30	10.256	1581	1586	1593	rVV	484580	628962	31.78%	5.490%
31	10.366	1597	1604	1616	rVB	1529362	1979236	100.00%	17.277%
32	10.707	1654	1660	1667	rVB	395730	499130	25.22%	4.357%
33	11.024	1706	1712	1718	rBV	20292	24892	1.26%	0.217%
34	11.146	1726	1732	1743	rBV	397422	495950	25.06%	4.329%

LSC Area Percent Report

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ALS Vial : 41 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Title : SW846 8260

35	11.366	1763	1768	1774	rVB	44770	56882	2.87%	0.497%
36	11.439	1774	1780	1788	rBV	205132	375474	18.97%	3.278%
37	11.512	1788	1792	1799	rVB	105317	129174	6.53%	1.128%
38	11.677	1814	1819	1825	rBV	91635	117832	5.95%	1.029%
39	11.817	1836	1842	1848	rBV	377764	473101	23.90%	4.130%
40	12.085	1880	1886	1892	rBV	578132	698731	35.30%	6.099%
41	12.152	1892	1897	1902	rVB	97970	122839	6.21%	1.072%
42	12.304	1917	1922	1930	rBV2	135281	189994	9.60%	1.659%
43	12.378	1930	1934	1941	rVB3	30063	45012	2.27%	0.393%
44	12.591	1964	1969	1971	rBV	17378	21877	1.11%	0.191%
45	12.676	1978	1983	1986	rBV	25936	32066	1.62%	0.280%
46	12.762	1992	1997	2005	rBV2	24859	33130	1.67%	0.289%
47	13.024	2037	2040	2046	rVB	23591	27015	1.36%	0.236%
48	13.231	2069	2074	2079	rVB	23718	28821	1.46%	0.252%
49	13.359	2090	2095	2100	rVB2	41603	56445	2.85%	0.493%
50	13.841	2168	2174	2181	rBV	162387	199850	10.10%	1.745%
51	14.706	2311	2316	2322	rVB	24345	29979	1.51%	0.262%

Sum of corrected areas: 11455570

LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
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Operator : JC/MD
Sample : J2132-05 50X
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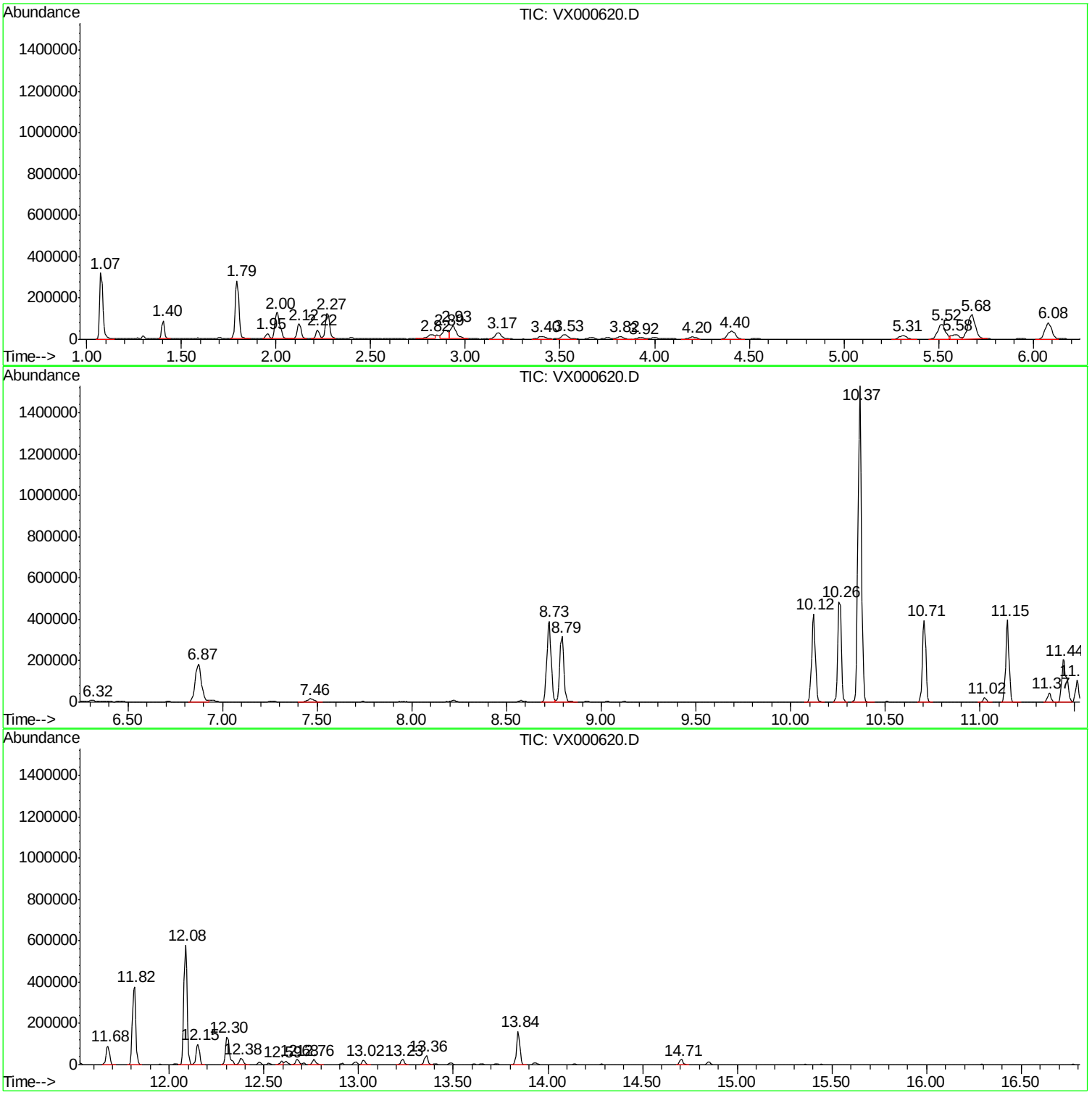
ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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



Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
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Misc : 5.0mL/MSVOA_X/WATER
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Quant Title : SW846 8260

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

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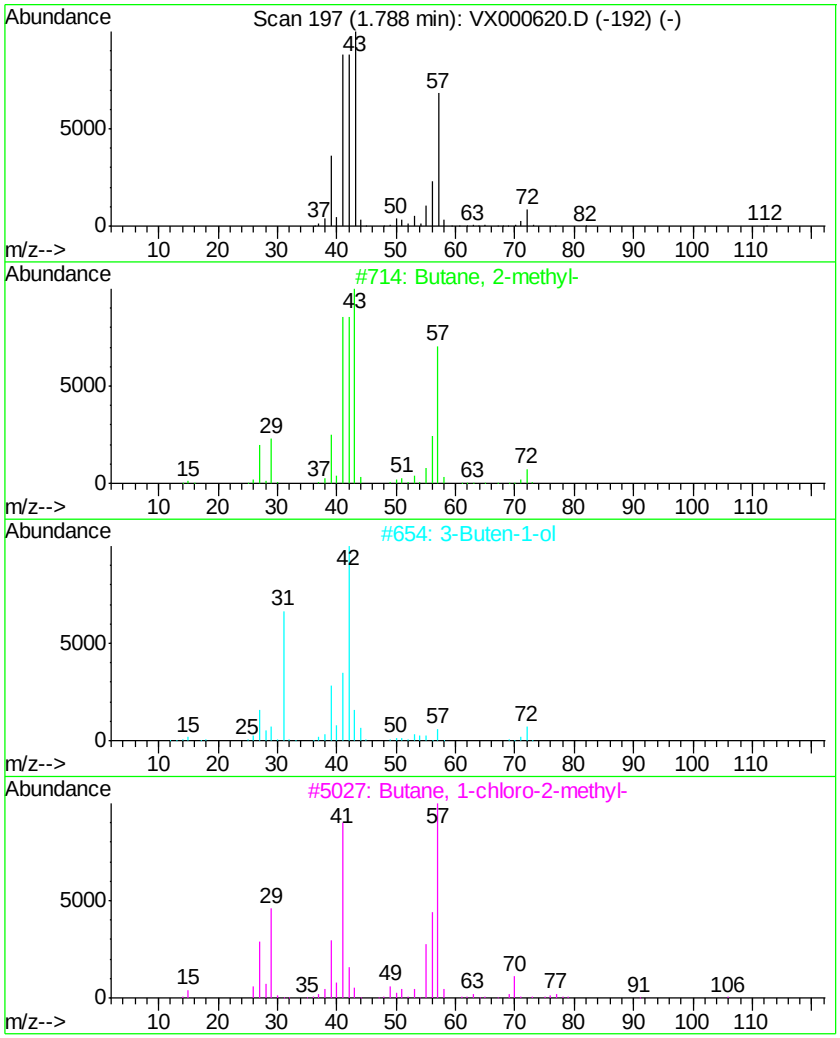
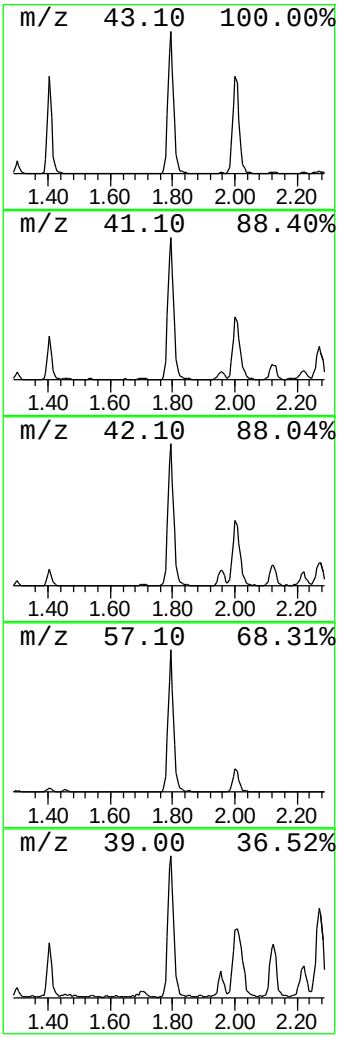
Peak Number 2 Butane, 2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	58.86 ug/l	388631	Pentafluorobenzene	5.68

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	43
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	35
4	Pentane	72	C5H12	000109-66-0	28
5	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
Sample : J2132-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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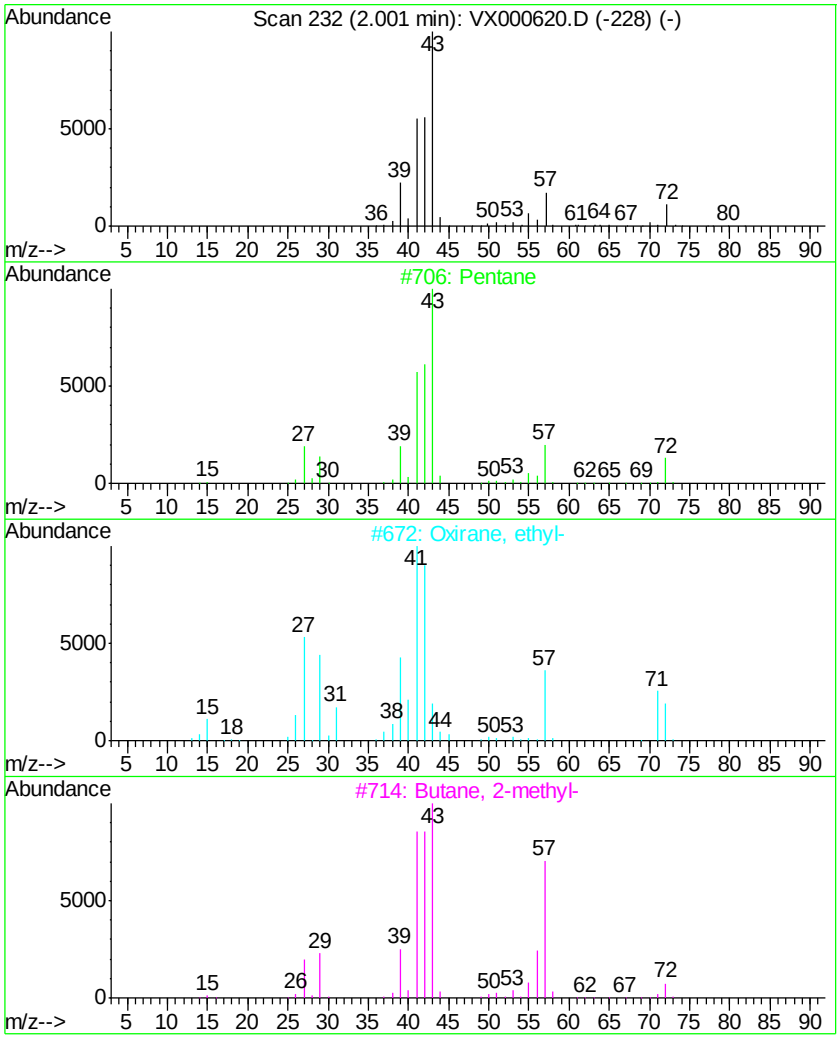
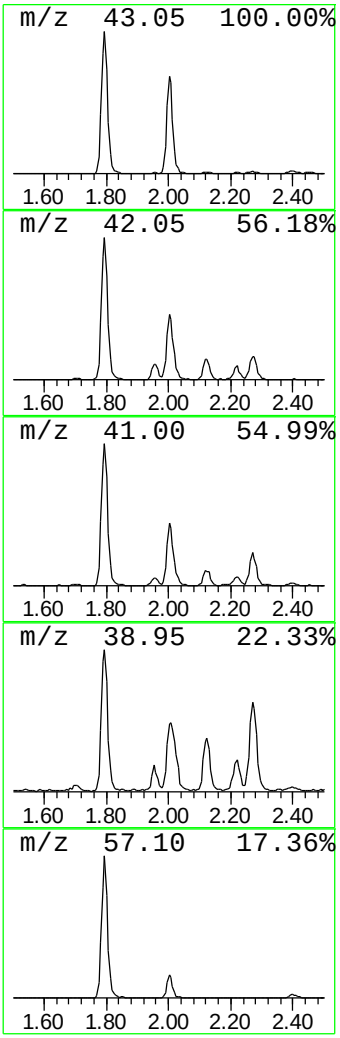
Peak Number 3 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	35.93 ug/l	237249	Pentafluorobenzene	5.68

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	Butane, 2-methyl-	72	C5H12	000078-78-4	33
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
5	Butanal, 2-ethyl-	100	C6H12O	000097-96-1	9





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
Sample : J2132-05 50X
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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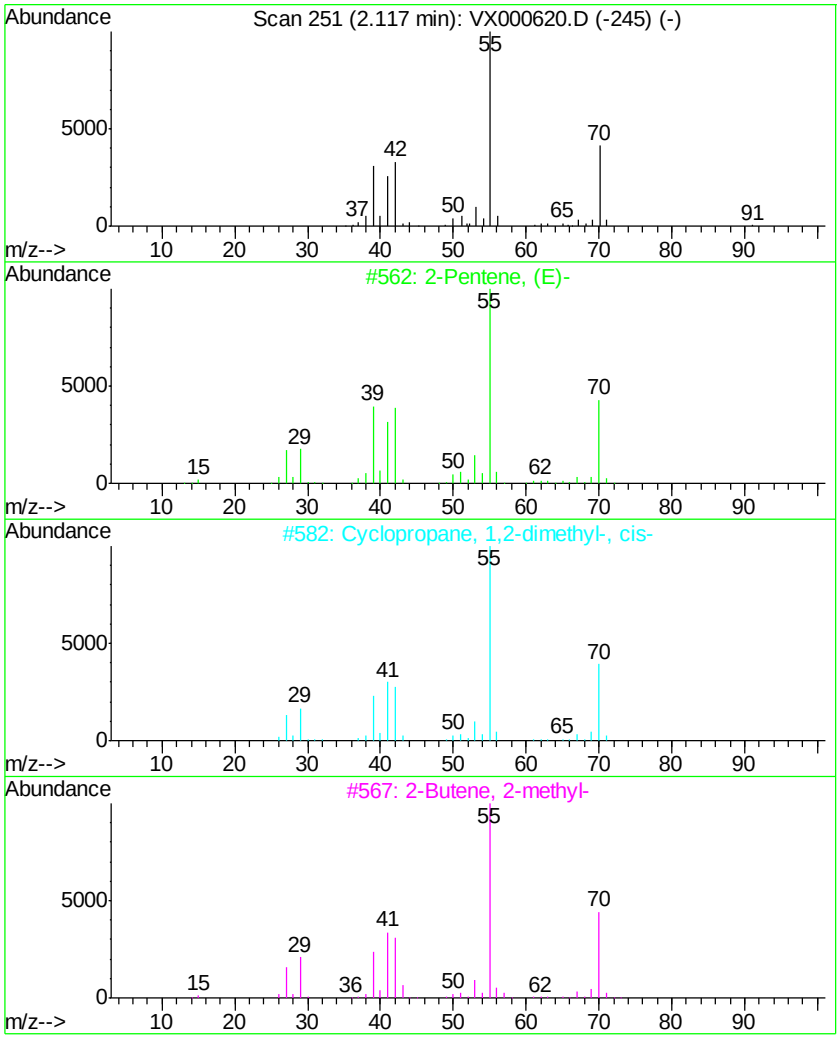
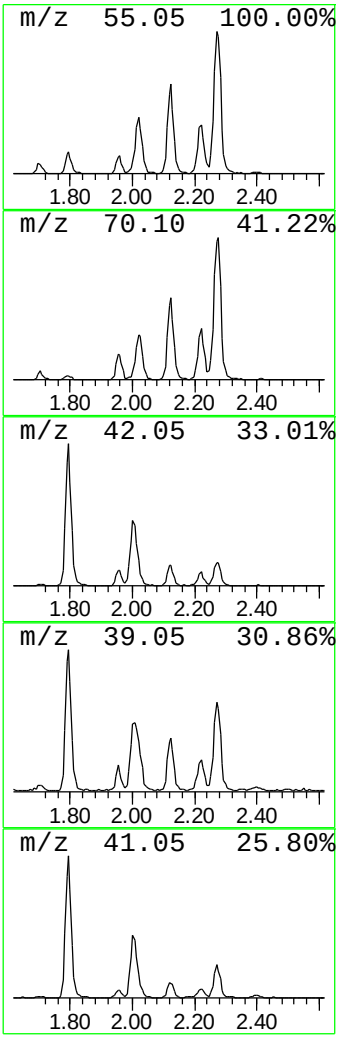
Peak Number 4 2-Pentene, (E)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.12	16.33 ug/l	107817	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (E)-	70	C5H10	000646-04-8	93
2	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
3	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
4	2-Methyl-1-butene	70	C5H10	000563-46-2	87
5	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	86





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ALS Vial : 41 Sample Multiplier: 1

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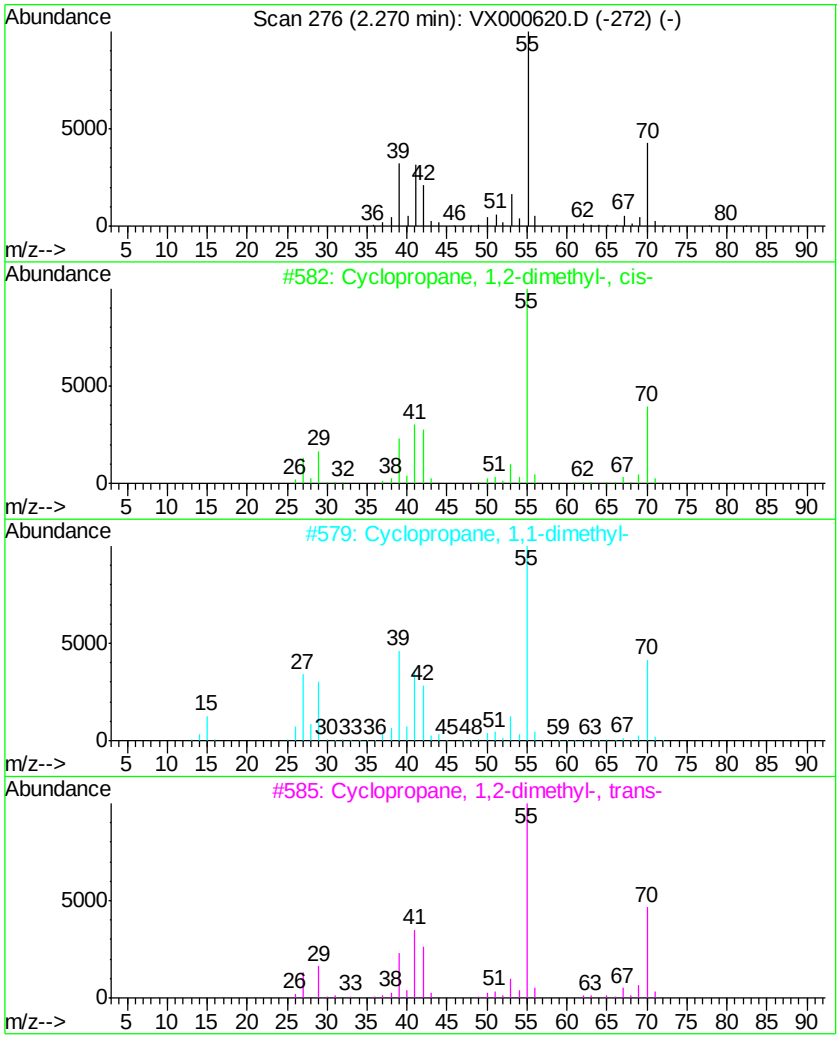
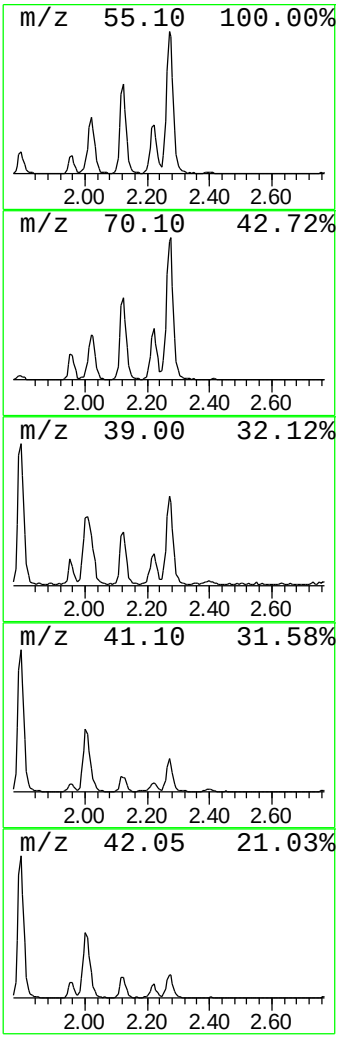
Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	27.97 ug/l	184651	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	87
3	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	78
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	78





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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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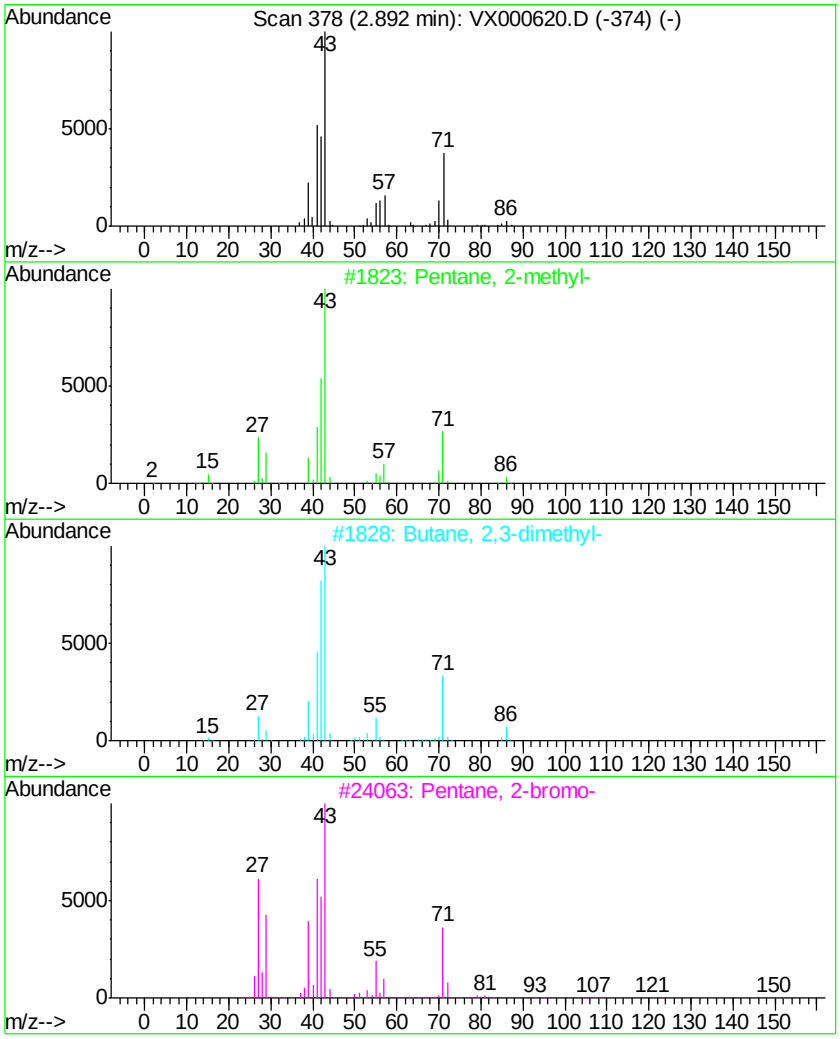
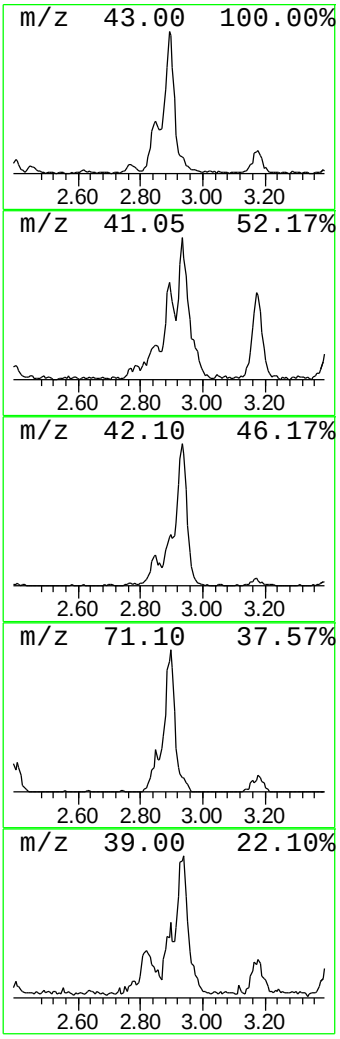
Peak Number 6 Pentane, 2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	14.91 ug/l	98418	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	86
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3	Pentane, 2-bromo-	150	C5H11Br	000107-81-3	45
4	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	36
5	Hydroxylamine, O-(3-methylbutyl)-	103	C5H13NO	019411-65-5	33





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Sample : J2132-05 50X
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ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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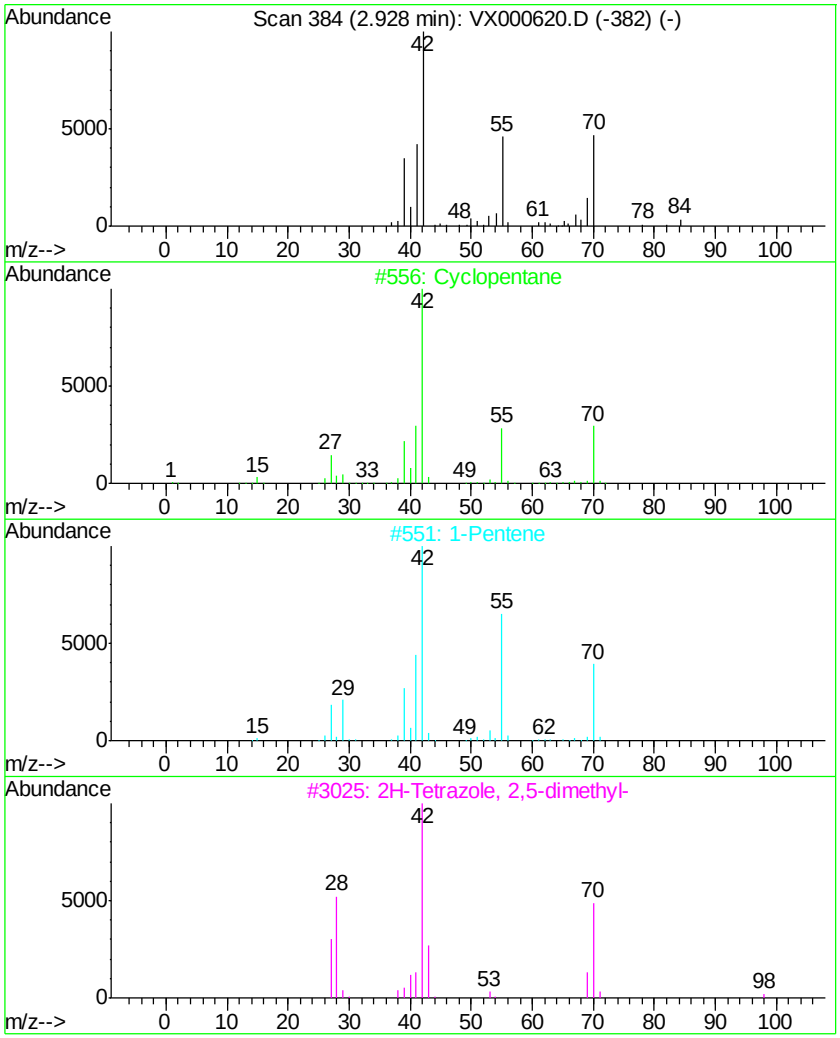
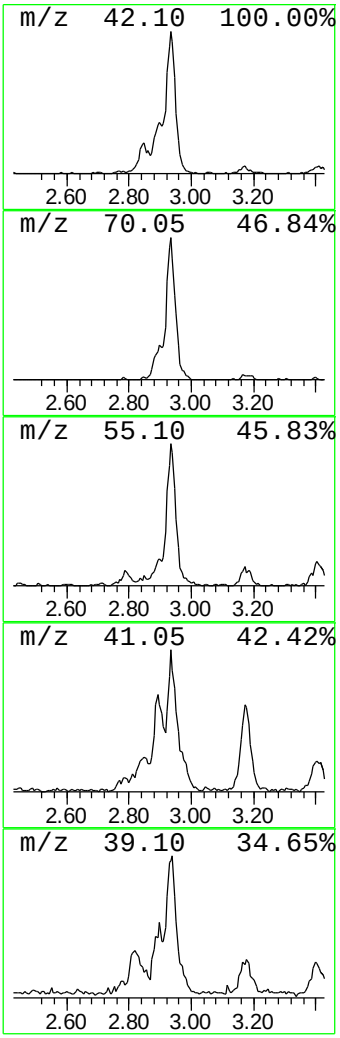
Peak Number 7 Cyclopentane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	21.12 ug/l	139447	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	72
2	1-Pentene	70	C5H10	000109-67-1	45
3	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	39
4	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	27
5	(Z)-1,3-Butadien-1-ol	70	C4H6O	070415-58-6	14





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Misc : 5.0mL/MSVOA_X/WATER
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

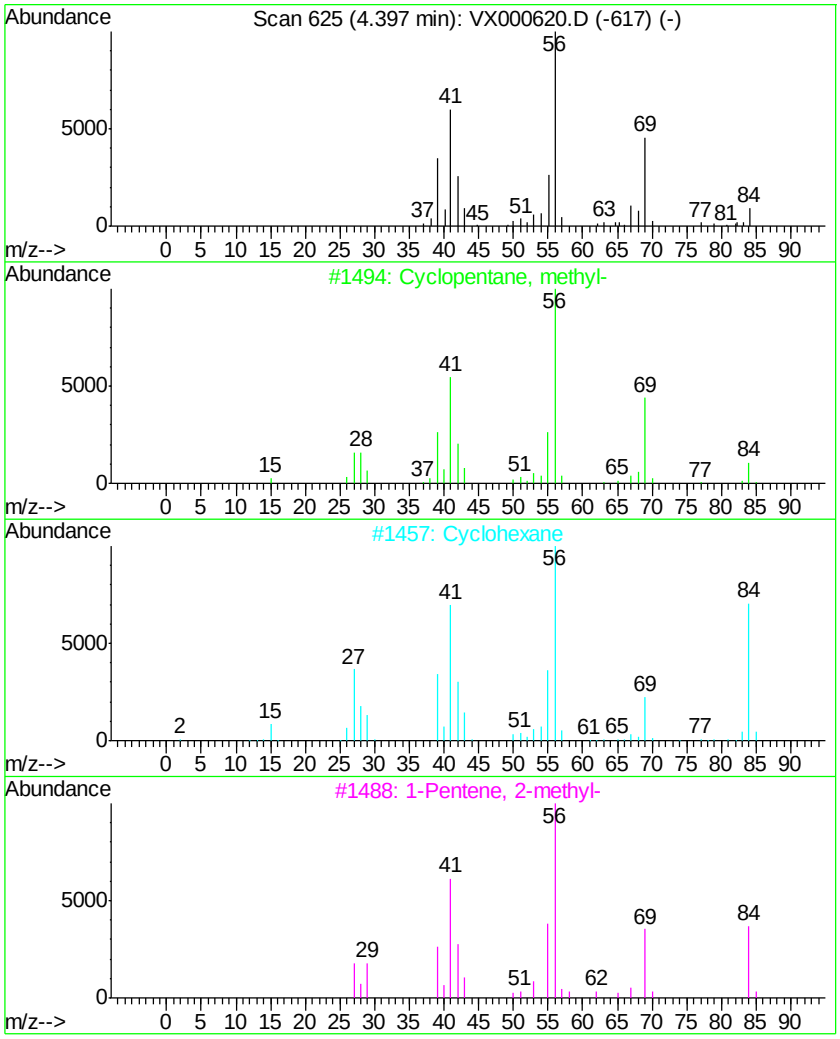
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

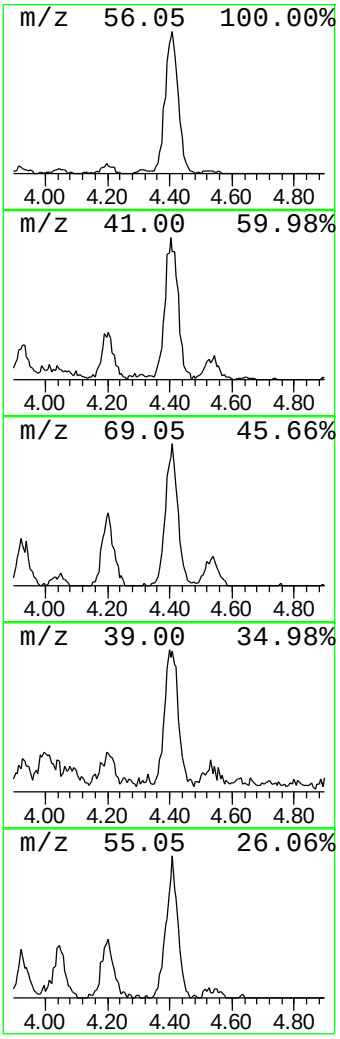
****

Peak Number 8 Cyclopentane, methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	17.88 ug/l	118068	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	87
2	Cyclohexane	84	C6H12	000110-82-7	72
3	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	72
4	Cyclobutane, butyl-	112	C8H16	013152-44-8	72
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59





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ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

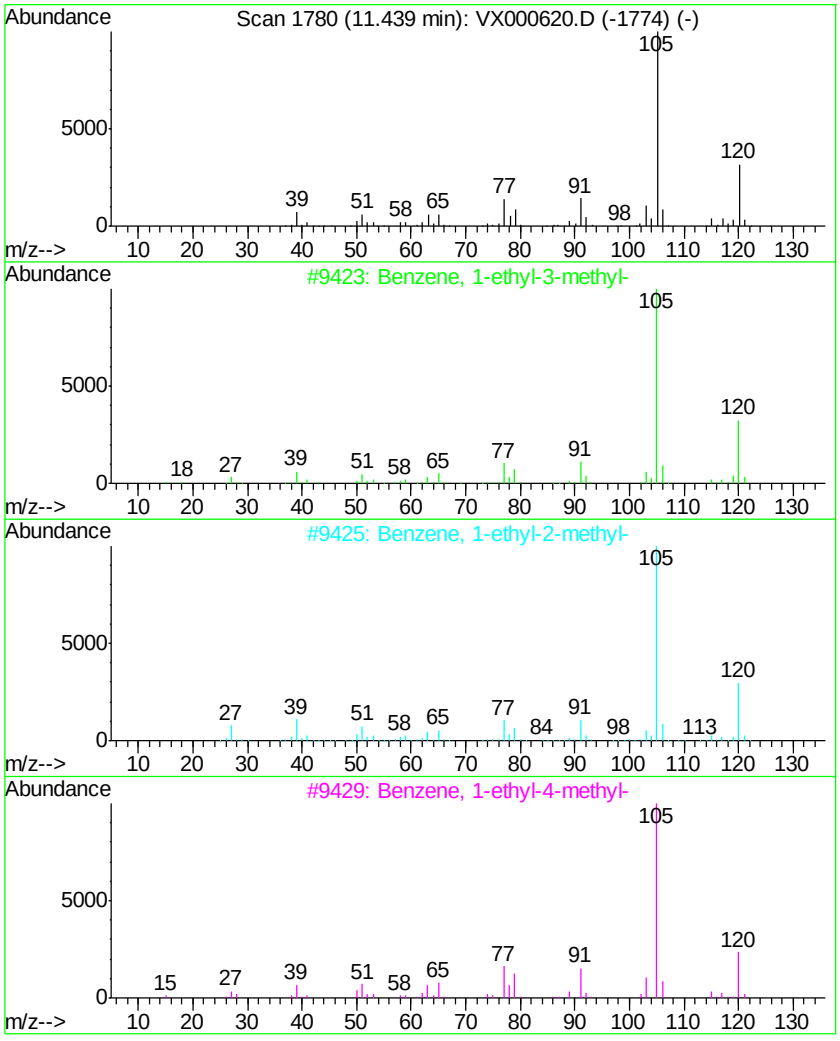
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

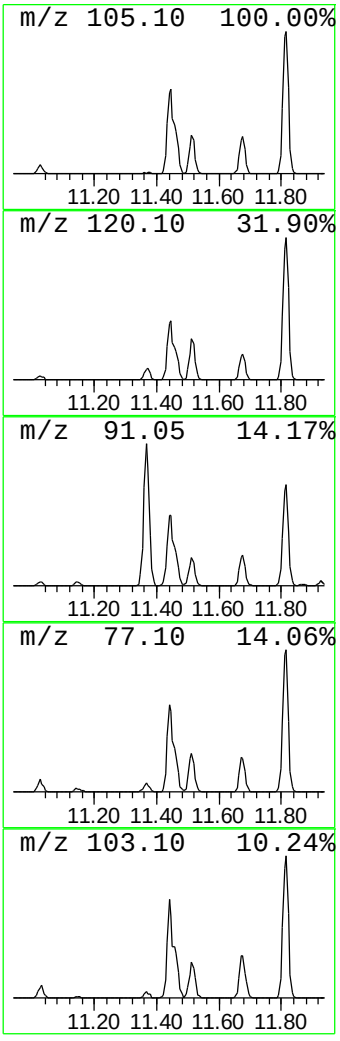
****

Peak Number 9 Benzene, 1-ethyl-3-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	26.87 ug/l	375474	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	97
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	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 : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
Sample : J2132-05 50X
Misc : 5.0mL/MSVOA_X/WATER
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Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.M
Quant Title : SW846 8260

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

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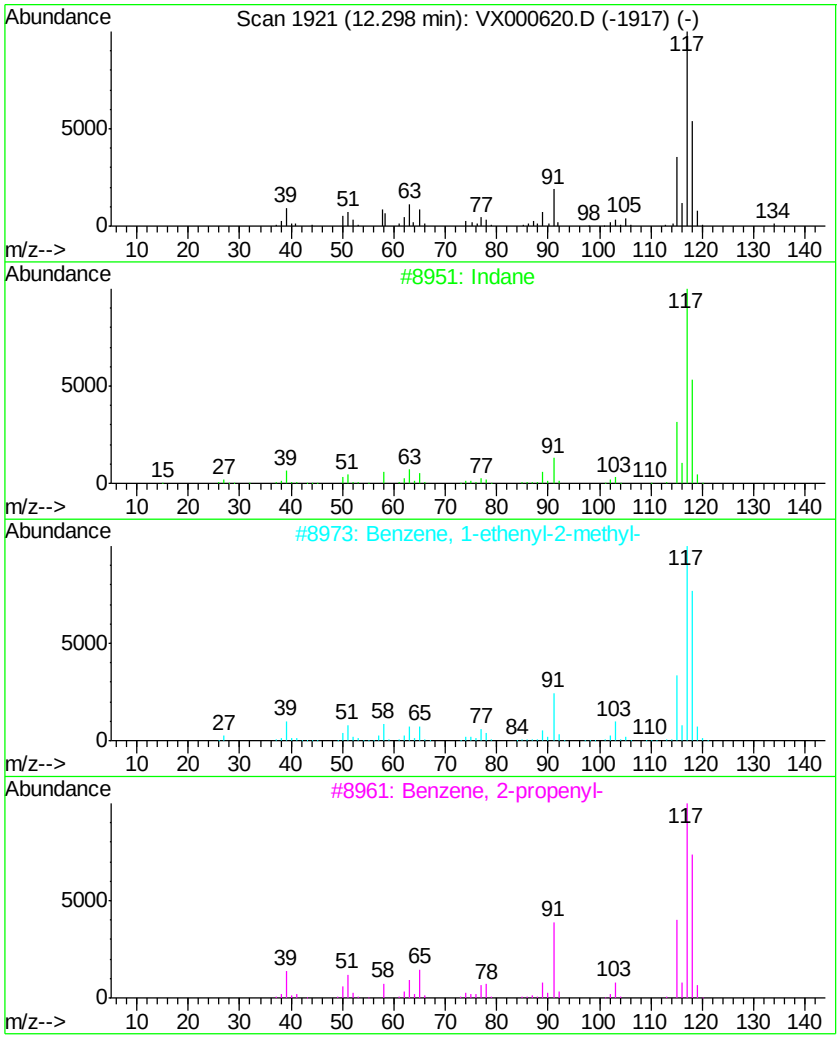
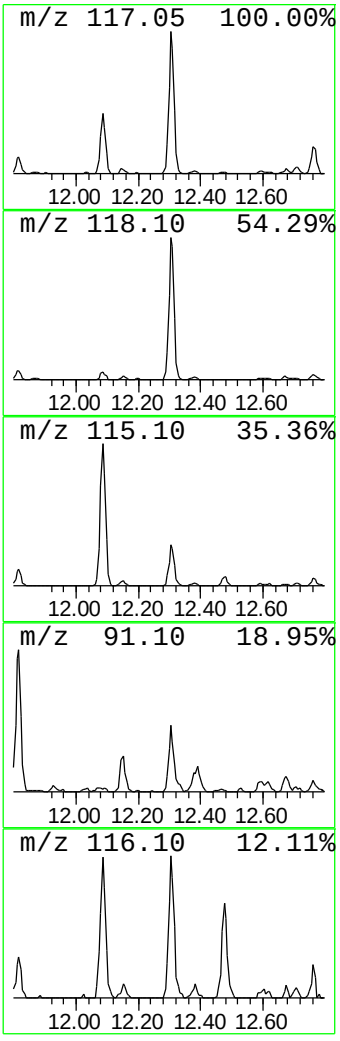
Peak Number 10 Indane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	13.60 ug/l	189994	1,4-Dichlorobenzene-d4	12.09

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	95
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	90
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	87
4	Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
5	Tetracyclo[3.3.1.0(2,8).0(4,6)]-...	118	C9H10	1000191-13-7	72





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000620.D
Acq On : 01 Apr 2018 03:38
Operator : JC/MD
Sample : J2132-05 50X
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 41 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_X\METHOD\82X032018W.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	58.9	ug/l	388631	1	5.68	330116	50.0
Pentane	2.00	35.9	ug/l	237249	1	5.68	330116	50.0
2-Pentene, (E)-	2.12	16.3	ug/l	107817	1	5.68	330116	50.0
Cyclopropane, 1,2...	2.27	28.0	ug/l	184651	1	5.68	330116	50.0
Pentane, 2-methyl-	2.89	14.9	ug/l	98418	1	5.68	330116	50.0
Cyclopentane	2.93	21.1	ug/l	139447	1	5.68	330116	50.0
Cyclopentane, met...	4.40	17.9	ug/l	118068	1	5.68	330116	50.0
Benzene, 1-ethyl-...	11.44	26.9	ug/l	375474	4	12.09	698731	50.0
Indane	12.30	13.6	ug/l	189994	4	12.09	698731	50.0