LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 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	90	rBV	373334	446658	5.67%	0.715%
2	1.404	130	134	139	rBV	161966	161390	2.05%	0.258%
3	1.794	192	198	212	rVB	1615881	2179049	27.64%	3.487%
4	2.001	227	232	245	rVB	589834	879966	11.16%	1.408%
5	2.123	245	252	258	rBV	120491	170372	2.16%	0.273%
6	2.270	272	276	287	rVB	166790	256899	3.26%	0.411%
7	2.398	288	297	303	rBV	69420	138960	1.76%	0.222%
8	2.849	352	371	374	rBV2	199224	552145	7.00%	0.884%
9	2.892	374	378	382	rVV	499237	1034488	13.12%	1.656%
10	2.934	382	385	404	rVB2	365038	800613	10.15%	1.281%
11	3.172	415	424	436	rVB	401256	910773	11.55%	1.458%
12	3.526	471	482	491	rBV2	101821	238627	3.03%	0.382%
13	3.818	524	530	540	rVB2	47186	116890	1.48%	0.187%
14	3.928	540	548	554	rBV2	39704	102237	1.30%	0.164%
15	4.196	585	592	602	rVB3	39792	101979	1.29%	0.163%
16	4.403	616	626	639	rVB	445450	1291971	16.39%	2.068%
17	5.306	768	774	786	rVB2	31695	101354	1.29%	0.162%
18	5.513	794	808	812	rBV	84516	227705	2.89%	0.364%
19	5.586	812	820	828	rVV3	189058	562108	7.13%	0.900%
20	5.672	828	834	841	rVV	91025	217526	2.76%	0.348%
21	5.934	866	877	892	rBV5	66624	211674	2.68%	0.339%
22	6.080	892	901	907	rBV	87776	226093	2.87%	0.362%
23	6.153	907	913	922	rVB2	36293	85697	1.09%	0.137%
24	6.269	922	932	935	rBV4	57781	153703	1.95%	0.246%
25	6.367	942	948	957	rVB5	69922	197473	2.50%	0.316%
26	6.464	957	964	977	rVB2	50392	145917	1.85%	0.234%
27	6.873	1022	1031	1038	rBV	212335	514219	6.52%	0.823%
28	7.470	1114	1129	1140	rBV3	169694	457947	5.81%	0.733%
29	8.183	1238	1246	1249	rBV	40670	80997	1.03%	0.130%
30	8.586	1306	1312	1320	rVB4	56593	131154	1.66%	0.210%
31	8.726	1329	1335	1340	rVB	434952	666988	8.46%	1.067%
32	8.793	1340	1346	1352	rBV	694871	1023852	12.99%	1.639%
33	10.122	1554	1564	1569	rBV	488288	682089	8.65%	1.092%
34	10.262	1581	1587	1598	rBV	4235136	5387898	68.34%	8.623%

LSC Area Percent Report

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Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 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

35	10.366	1598	1604	1612	rVB	6046967	7883996	100.00%	12.617%
36	10.707	1654	1660	1671	rVB	3156669	3897993	49.44%	6.238%
37	11.024	1706	1712	1719	rBV	387485	485379	6.16%	0.777%
38	11.146	1723	1732	1737	rBV	514084	645762	8.19%	1.033%
39	11.366	1758	1768	1775	rBV	854301	1032025	13.09%	1.652%
40	11.439	1775	1780	1788	rVV	1592474	2838483	36.00%	4.543%
41	11.512	1788	1792	1798	rVB	717629	850877	10.79%	1.362%
42	11.677	1813	1819	1827	rBV	1373199	1664879	21.12%	2.664%
43	11.817	1836	1842	1847	rVB	5351520	6190719	78.52%	9.907%
44	11.951	1862	1864	1872	rVB	71246	90704	1.15%	0.145%
45	12.030	1872	1877	1881	rBV	98959	128471	1.63%	0.206%
46	12.085	1881	1886	1891	rVB	771398	977055	12.39%	1.564%
47	12.152	1891	1897	1902	rBV	913191	1097654	13.92%	1.757%
48	12.304	1916	1922	1930	rBV2	1688344	2536426	32.17%	4.059%
49	12.378	1930	1934	1942	rVB3	397396	644946	8.18%	1.032%
50	12.475	1944	1950	1954	rBV2	142609	201593	2.56%	0.323%
51	12.524	1954	1958	1964	rVB	116981	143529	1.82%	0.230%
52	12.597	1964	1970	1972	rBV	449527	615265	7.80%	0.985%
53	12.615	1972	1973	1978	rVB	241180	222676	2.82%	0.356%
54	12.676	1978	1983	1986	rBV	732064	836749	10.61%	1.339%
55	12.707	1986	1988	1993	rVV	198292	227051	2.88%	0.363%
56	12.762	1993	1997	2005	rVV	662049	885898	11.24%	1.418%
57	12.914	2017	2022	2026	rVB2	75204	107872	1.37%	0.173%
58	12.987	2026	2034	2037	rBV	458722	567713	7.20%	0.909%
59	13.024	2037	2040	2046	rVB	547944	668070	8.47%	1.069%
60	13.091	2046	2051	2056	rBV3	50654	109287	1.39%	0.175%
61	13.231	2070	2074	2079	rVB	610979	740545	9.39%	1.185%
62	13.359	2090	2095	2100	rVB2	1147104	1512143	19.18%	2.420%
63	13.487	2112	2116	2124	rVB	178198	230810	2.93%	0.369%
64	13.566	2124	2129	2132	rBV2	70271	100622	1.28%	0.161%
65	13.609	2132	2136	2139	rVV	167998	234416	2.97%	0.375%
66	13.652	2139	2143	2149	rVV3	163021	320215	4.06%	0.512%
67	13.731	2149	2156	2161	rVB2	151900	317910	4.03%	0.509%
68	13.841	2167	2174	2180	rBV	1417484	1750636	22.20%	2.802%
69	13.932	2184	2189	2194	rVV	168958	227662	2.89%	0.364%
70	13.993	2194	2199	2203	rVV2	68052	94372	1.20%	0.151%
71	14.140	2218	2223	2228	rBV	104544	132638	1.68%	0.212%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 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

72	14.280	2242	2246	2252	rBV	82919	134203	1.70%	0.215%
73	14.707	2312	2316	2326	rVB	114712	169709	2.15%	0.272%
74	14.847	2334	2339	2349	rVB	403615	511808	6.49%	0.819%

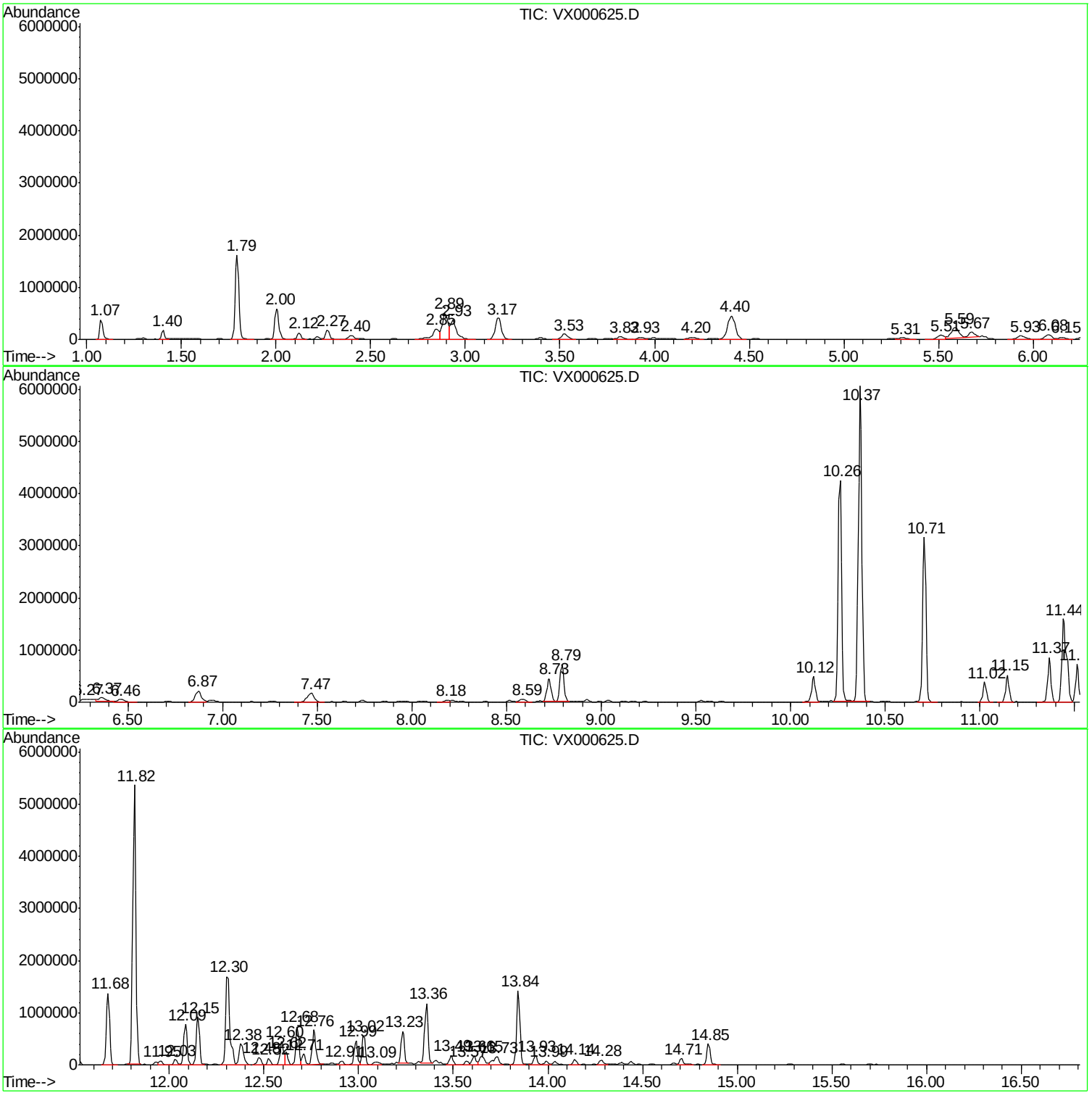
Sum of corrected areas: 62486172

LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 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 : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

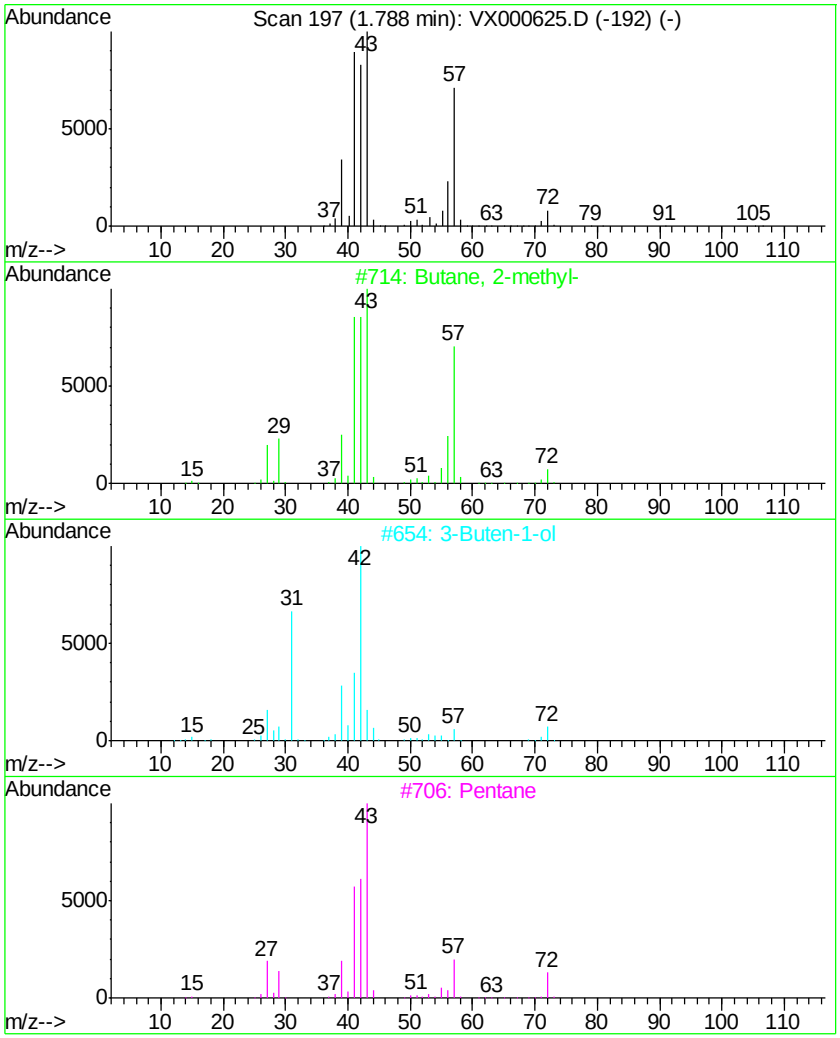
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

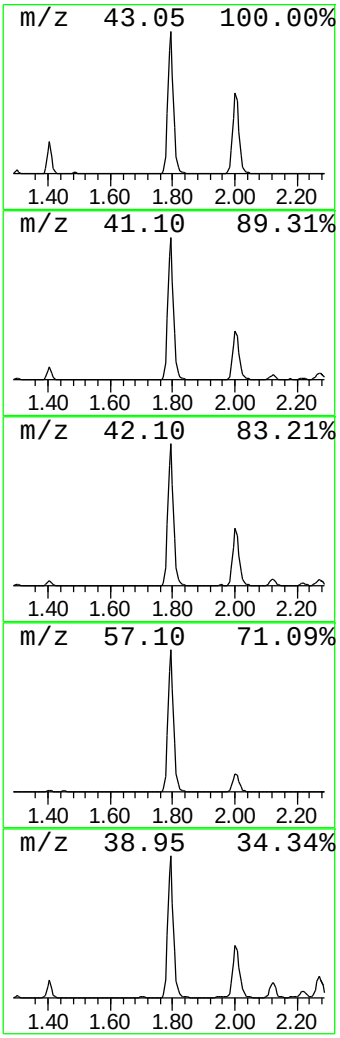
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	500.87 ug/l	2179050	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	47
3	Pentane	72	C5H12	000109-66-0	36
4	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	27
5	1-Butene	56	C4H8	000106-98-9	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

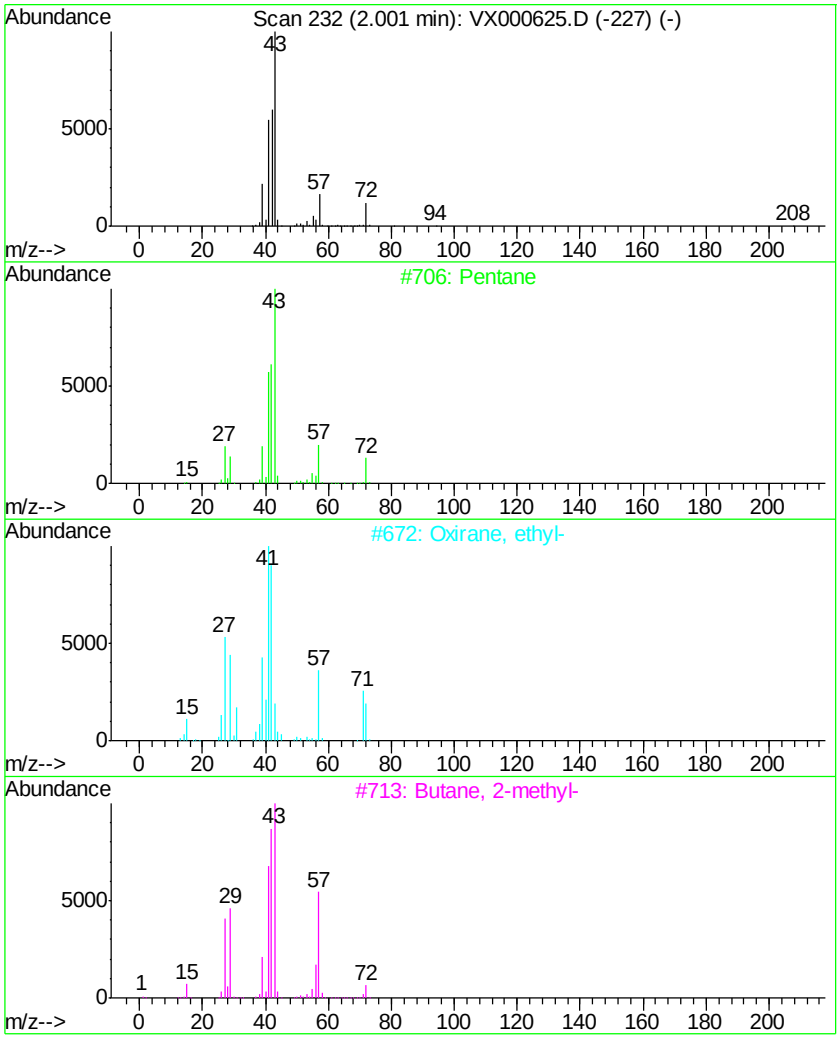
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

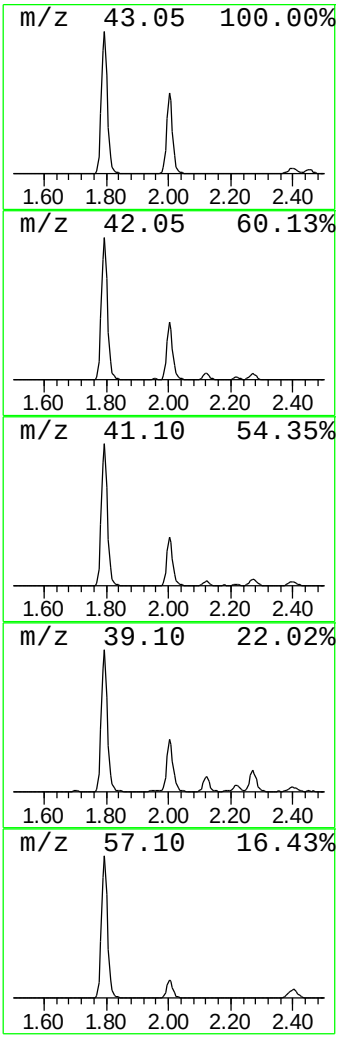
****

Peak Number 3 Pentane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	202.27 ug/l	879966	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	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	Cyclobutylamine	71	C4H9N	002516-34-9	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

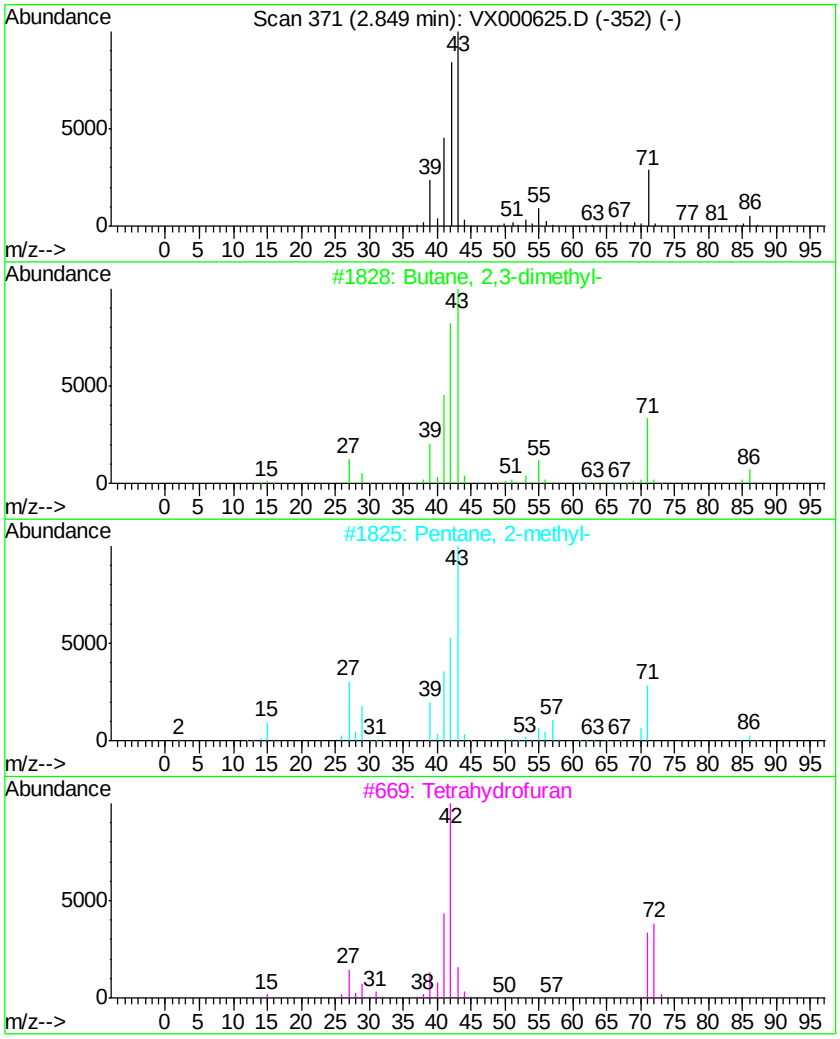
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

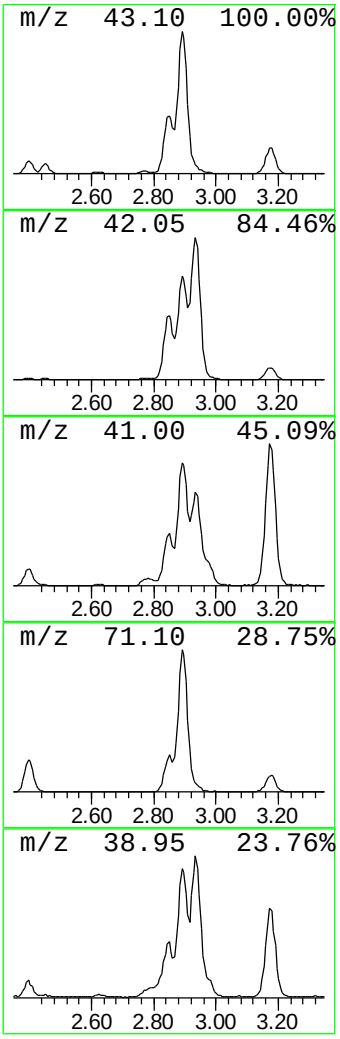
****

Peak Number 4 Butane, 2,3-dimethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.85	126.92 ug/l	552145	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	91
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	50
3	Tetrahydrofuran	72	C4H8O	000109-99-9	38
4	Pentane	72	C5H12	000109-66-0	36
5	Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	22





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

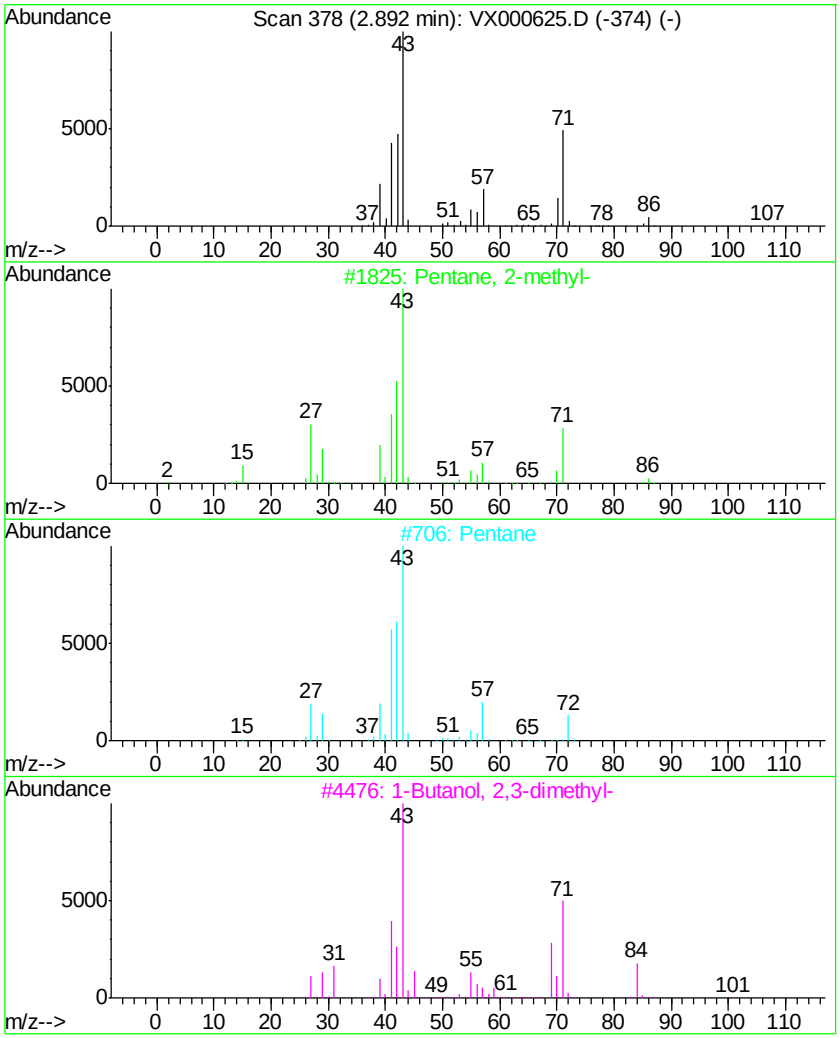
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

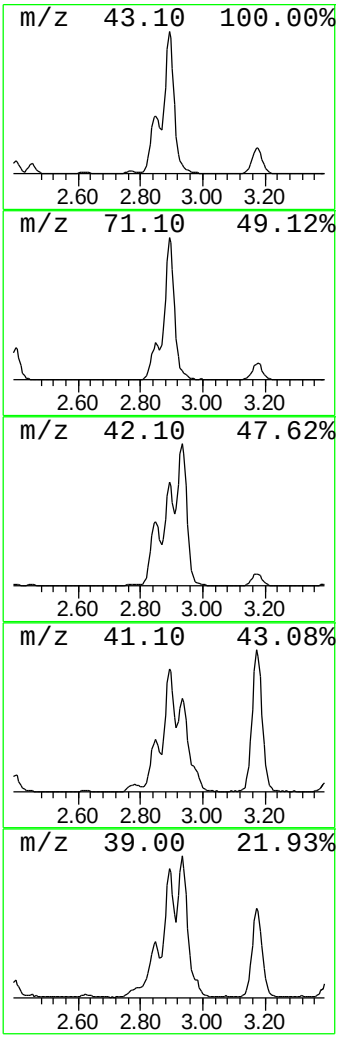
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	237.79 ug/l	1034490	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	91
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 : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

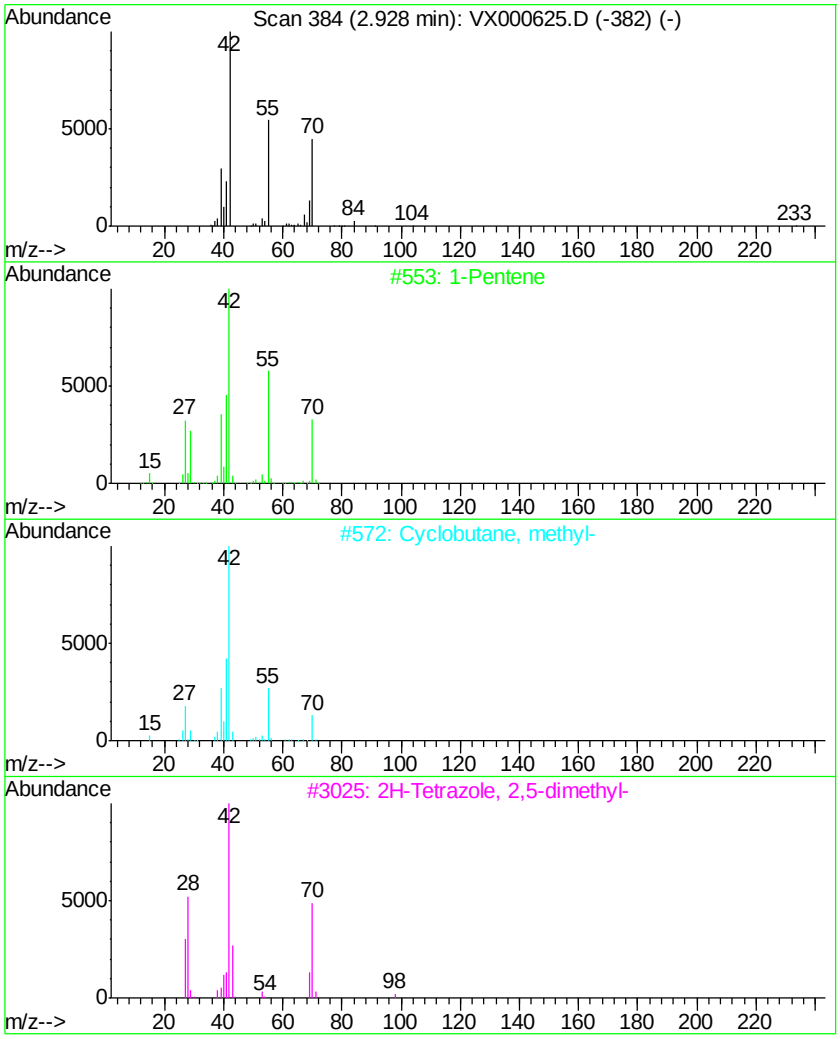
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

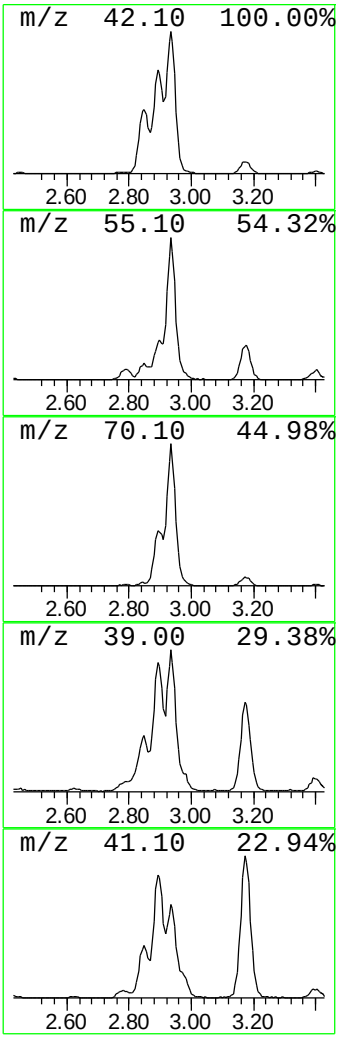
****

Peak Number 6 1-Pentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	184.03 ug/l	800613	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	72
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	50
4	2-Pentene	70	C5H10	000109-68-2	37
5	2-Pentene, (E)-	70	C5H10	000646-04-8	37





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

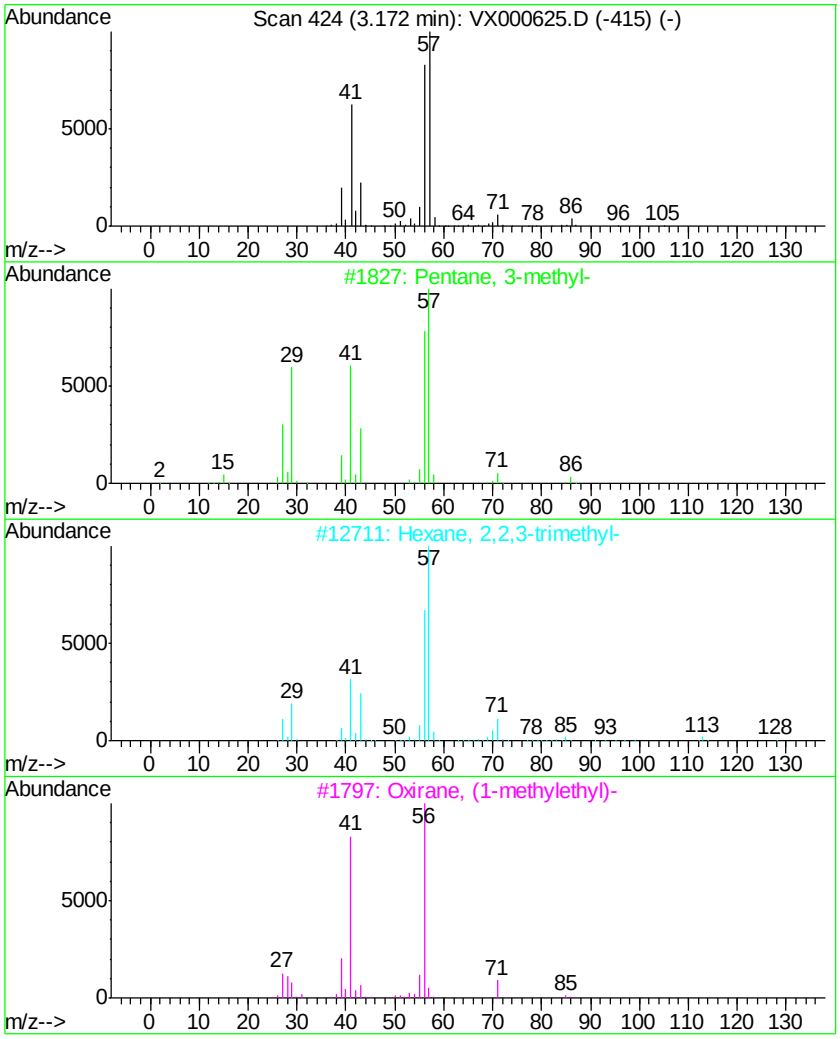
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

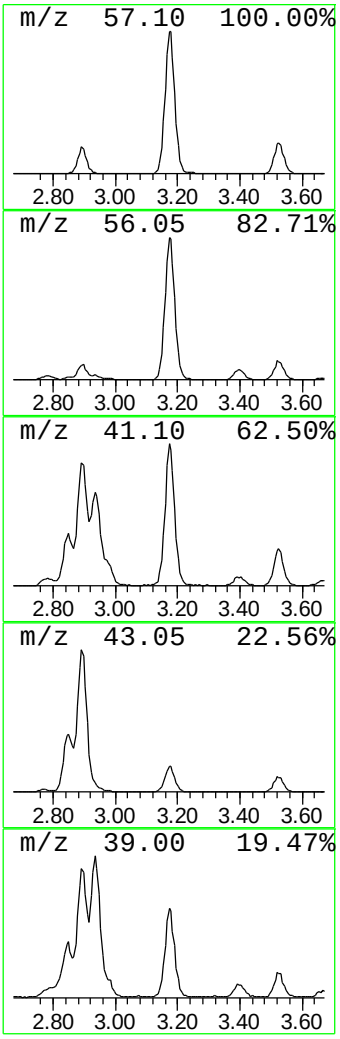
****

Peak Number 7 Pentane, 3-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	209.35 ug/l	910773	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	90
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
4	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	42





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

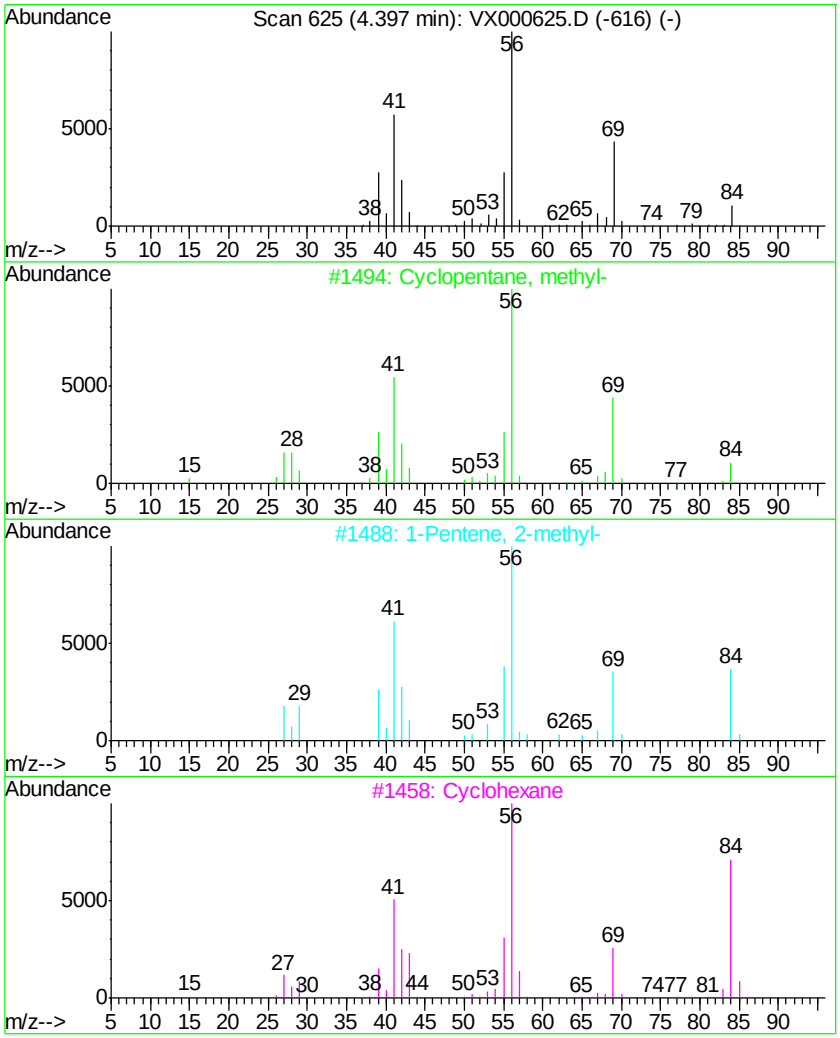
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

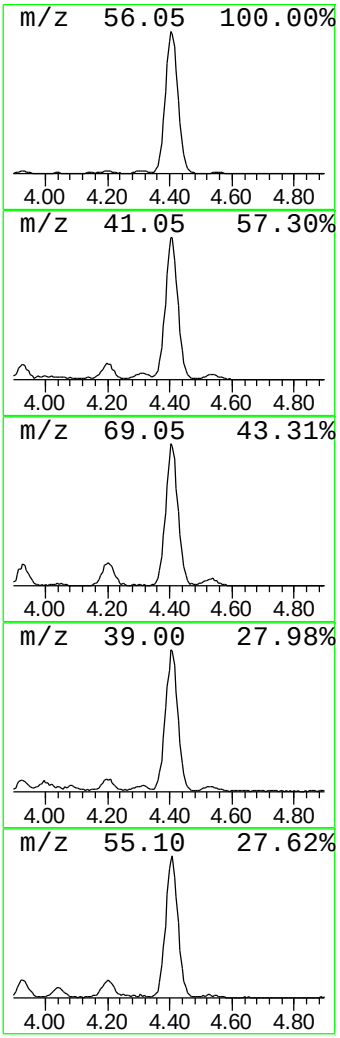
****

Peak Number 8 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	296.97 ug/l	1291970	Pentafluorobenzene	5.68

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	86
3	Cyclohexane	84	C6H12	000110-82-7	78
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	Cyclobutane	56	C4H8	000287-23-0	53





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

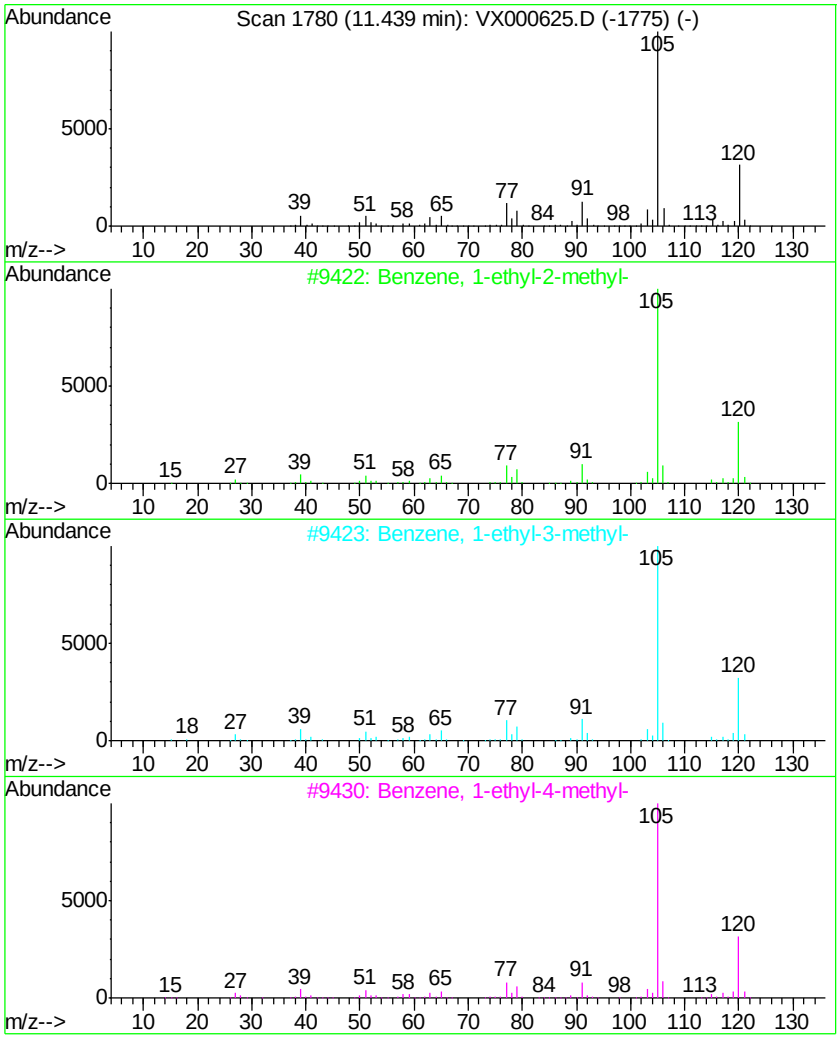
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

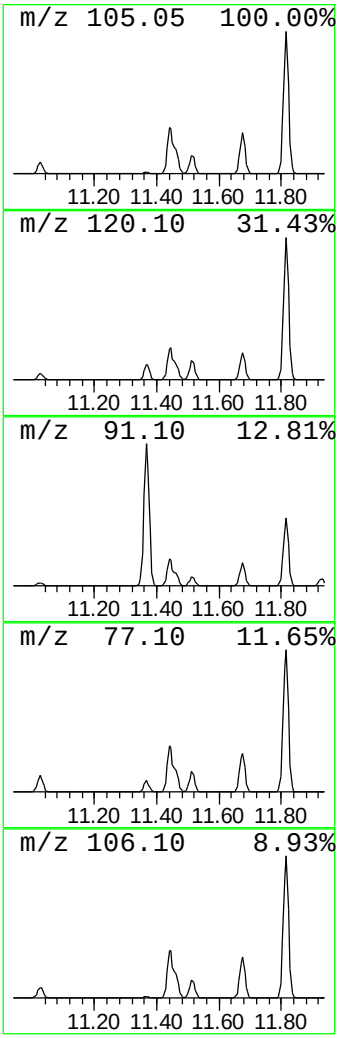
****

Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.44	145.26 ug/l	2838480	1,4-Dichlorobenzene-d4	12.09

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	94
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 : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 46 Sample Multiplier: 1

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

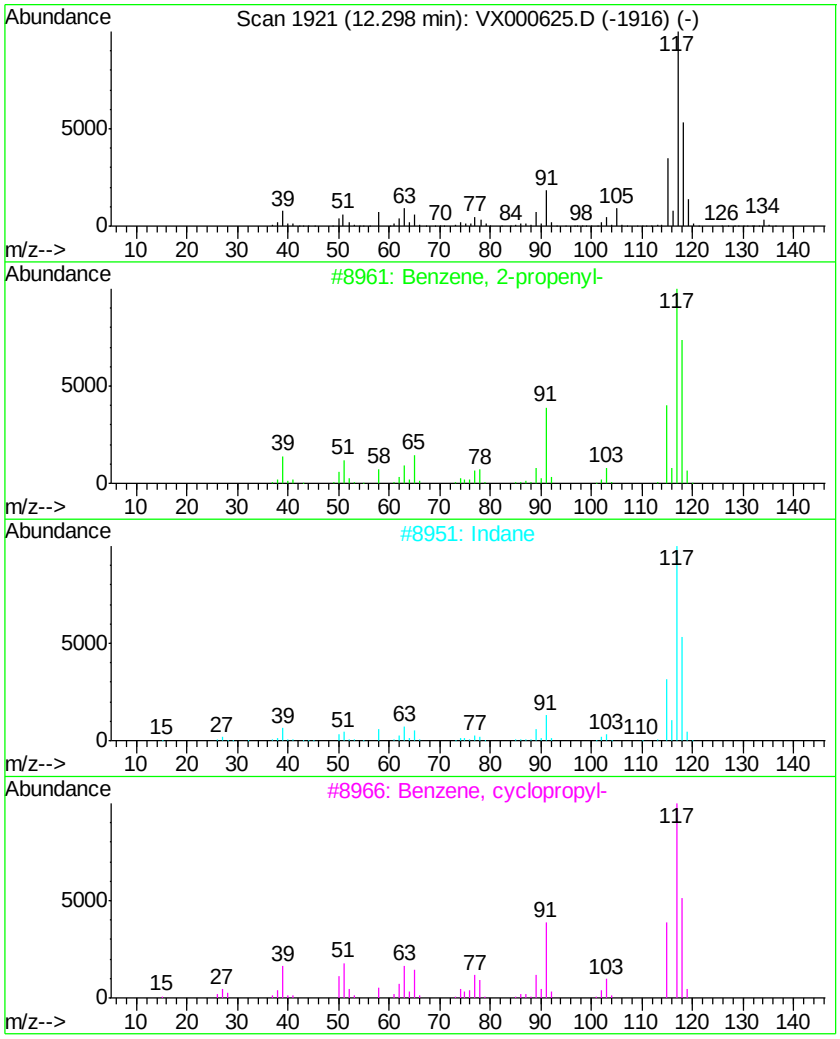
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

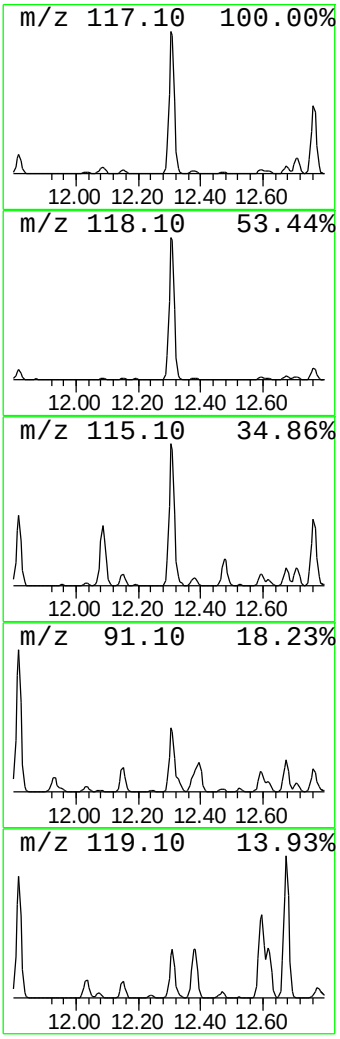
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.30	129.80 ug/l	2536430	1,4-Dichlorobenzene-d4	12.09

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 : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000625.D
Acq On : 01 Apr 2018 05:45
Operator : JC/MD
Sample : J2132-02
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 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	500.9	ug/l	2179050	1	5.68	217526	50.0
Pentane	2.00	202.3	ug/l	879966	1	5.68	217526	50.0
Butane, 2,3-dimet...	2.85	126.9	ug/l	552145	1	5.68	217526	50.0
Pentane, 2-methyl-	2.89	237.8	ug/l	1034490	1	5.68	217526	50.0
1-Pentene	2.93	184.0	ug/l	800613	1	5.68	217526	50.0
Pentane, 3-methyl-	3.17	209.3	ug/l	910773	1	5.68	217526	50.0
Cyclopentane, met...	4.40	297.0	ug/l	1291970	1	5.68	217526	50.0
Benzene, 1-ethyl-...	11.44	145.3	ug/l	2838480	4	12.09	977055	50.0
Benzene, 2-propenyl-	12.30	129.8	ug/l	2536430	4	12.09	977055	50.0