LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 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	91	rBV	424808	496987	11.11%	1.883%
2	1.300	114	117	130	rVB	226494	231158	5.17%	0.876%
3	1.404	130	134	140	rBV	1156067	1156975	25.86%	4.384%
4	1.703	177	183	192	rBV	46650	63264	1.41%	0.240%
5	1.794	192	198	212	rVV	3363204	4474038	100.00%	16.953%
6	2.001	227	232	247	rVB2	613110	1074871	24.02%	4.073%
7	2.123	247	252	258	rBV	172985	241937	5.41%	0.917%
8	2.221	263	268	271	rVV	78694	118949	2.66%	0.451%
9	2.270	271	276	287	rVV	289546	458461	10.25%	1.737%
10	2.398	287	297	302	rVV	60987	128655	2.88%	0.487%
11	2.453	302	306	313	rVB	50463	81481	1.82%	0.309%
12	2.843	352	370	374	rBV2	166234	568508	12.71%	2.154%
13	2.892	374	378	381	rVV	363171	696023	15.56%	2.637%
14	2.934	381	385	405	rVB	441794	1016647	22.72%	3.852%
15	3.172	415	424	437	rBV	285042	647868	14.48%	2.455%
16	3.398	452	461	470	rBV3	30168	74380	1.66%	0.282%
17	3.526	473	482	492	rVB3	35387	85193	1.90%	0.323%
18	3.928	539	548	554	rBV	30597	80556	1.80%	0.305%
19	3.995	554	559	568	rVB2	25948	64042	1.43%	0.243%
20	4.403	615	626	639	rVB	296417	860707	19.24%	3.261%
21	5.312	766	775	787	rVB2	23651	77196	1.73%	0.293%
22	5.513	794	808	813	rBV2	78481	225021	5.03%	0.853%
23	5.586	813	820	828	rVV	141327	428951	9.59%	1.625%
24	5.672	828	834	863	rVB2	122117	454504	10.16%	1.722%
25	5.934	865	877	891	rVB5	30165	100655	2.25%	0.381%
26	6.080	891	901	906	rBV	83003	215263	4.81%	0.816%
27	6.153	906	913	924	rVB	172731	436363	9.75%	1.653%
28	6.269	924	932	934	rBV4	30731	70307	1.57%	0.266%
29	6.354	944	946	958	rVB5	34856	98191	2.19%	0.372%
30	6.464	958	964	975	rVB2	27009	78700	1.76%	0.298%
31	6.873	1022	1031	1039	rBV	193581	473492	10.58%	1.794%
32	7.464	1117	1128	1140	rBV3	107308	280425	6.27%	1.063%
33	7.964	1197	1210	1217	rBV5	15378	49643	1.11%	0.188%
34	8.586	1306	1312	1319	rVB4	25387	58826	1.31%	0.223%

LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 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	8.720	1329	1334	1341	rVV	407949	652223	14.58%	2.471%
36	8.793	1341	1346	1352	rVB	199897	296090	6.62%	1.122%
37	10.122	1554	1564	1570	rBV	452593	623731	13.94%	2.363%
38	10.256	1581	1586	1592	rVB	281670	375391	8.39%	1.422%
39	10.366	1599	1604	1610	rVB	519893	687999	15.38%	2.607%
40	10.707	1654	1660	1670	rVB	156413	205368	4.59%	0.778%
41	11.024	1706	1712	1719	rBV	155354	195179	4.36%	0.740%
42	11.146	1726	1732	1737	rBV	416213	514924	11.51%	1.951%
43	11.366	1758	1768	1776	rBV	141830	176514	3.95%	0.669%
44	11.463	1776	1784	1788	rVV	160230	261625	5.85%	0.991%
45	11.512	1788	1792	1797	rVB	52488	64495	1.44%	0.244%
46	11.677	1813	1819	1826	rBV	438255	520374	11.63%	1.972%
47	11.817	1836	1842	1847	rVB	737653	899174	20.10%	3.407%
48	12.085	1881	1886	1892	rVB	605596	735903	16.45%	2.788%
49	12.152	1892	1897	1902	rBV	111396	137867	3.08%	0.522%
50	12.305	1915	1922	1930	rBV2	351021	523540	11.70%	1.984%
51	12.378	1930	1934	1943	rVB3	66196	125943	2.81%	0.477%
52	12.475	1943	1950	1955	rBV2	44581	63721	1.42%	0.241%
53	12.591	1964	1969	1972	rBV	114096	154502	3.45%	0.585%
54	12.676	1977	1983	1986	rBV	176500	212305	4.75%	0.804%
55	12.762	1992	1997	2005	rBV	234628	319573	7.14%	1.211%
56	12.987	2027	2034	2037	rBV	120623	152423	3.41%	0.578%
57	13.024	2037	2040	2047	rVB	179817	211133	4.72%	0.800%
58	13.231	2070	2074	2078	rVB	131329	150812	3.37%	0.571%
59	13.359	2090	2095	2100	rVB2	343438	438035	9.79%	1.660%
60	13.487	2112	2116	2120	rBV2	41962	52495	1.17%	0.199%
61	13.609	2132	2136	2139	rBV	38270	51290	1.15%	0.194%
62	13.646	2139	2142	2148	rVV2	36966	67622	1.51%	0.256%
63	13.731	2148	2156	2161	rVB2	44384	94184	2.11%	0.357%
64	13.841	2167	2174	2180	rBV	1171727	1395557	31.19%	5.288%
65	13.932	2185	2189	2195	rVB	82876	112648	2.52%	0.427%
66	14.707	2312	2316	2321	rVB	76045	96733	2.16%	0.367%
67	14.847	2334	2339	2347	rVB	117468	153206	3.42%	0.581%

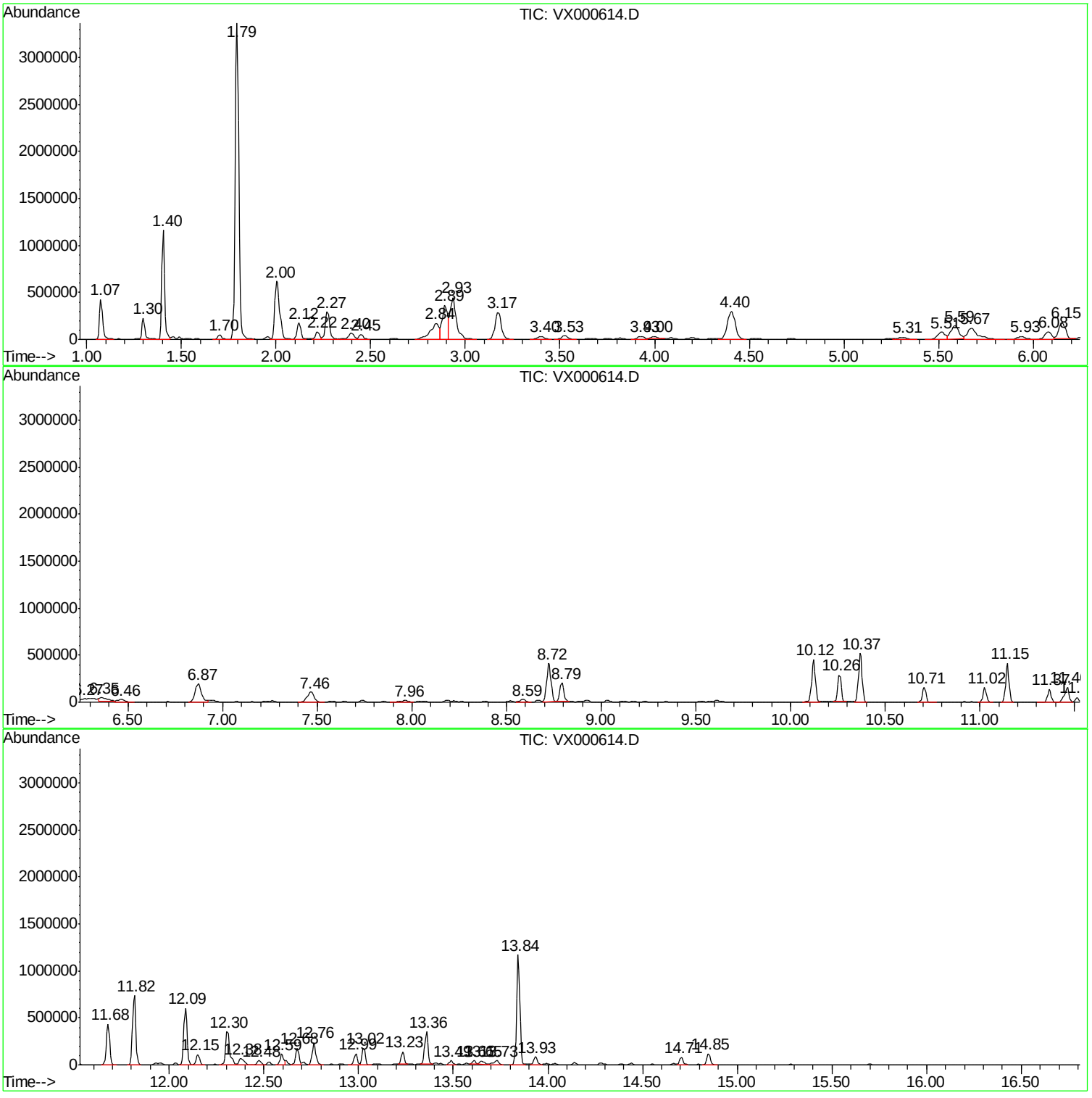
Sum of corrected areas: 26390816

LSC Report - Integrated Chromatogram

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 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



Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

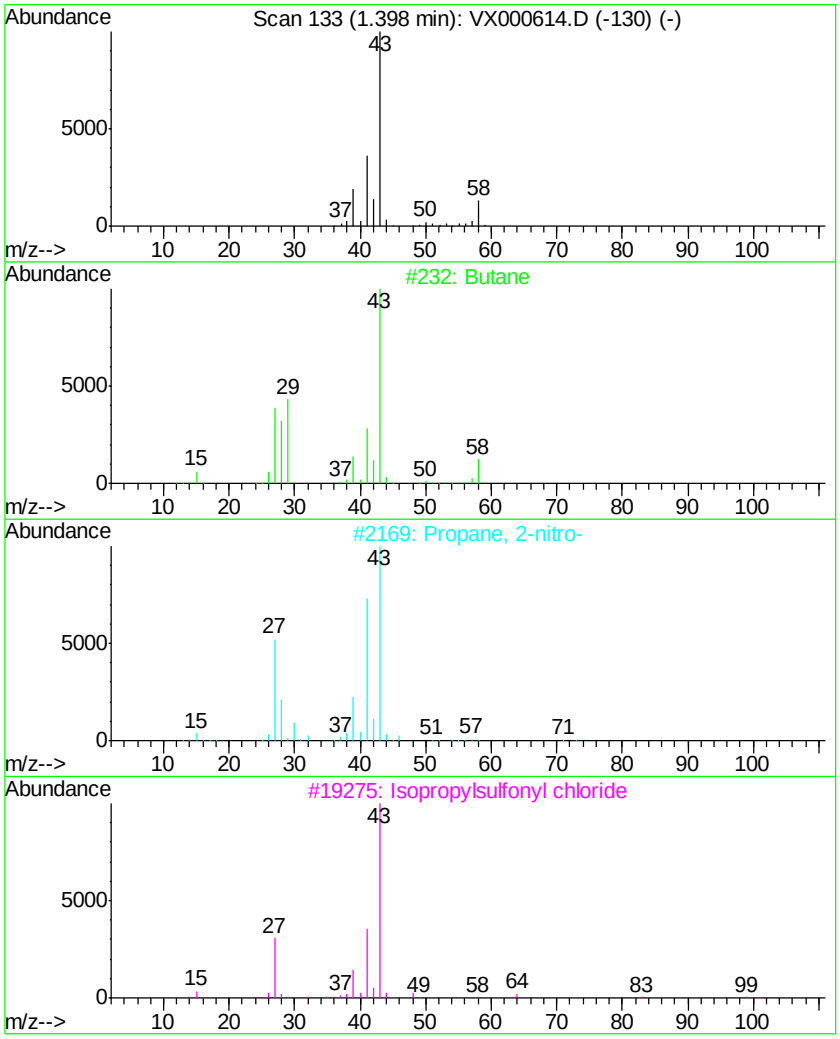
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

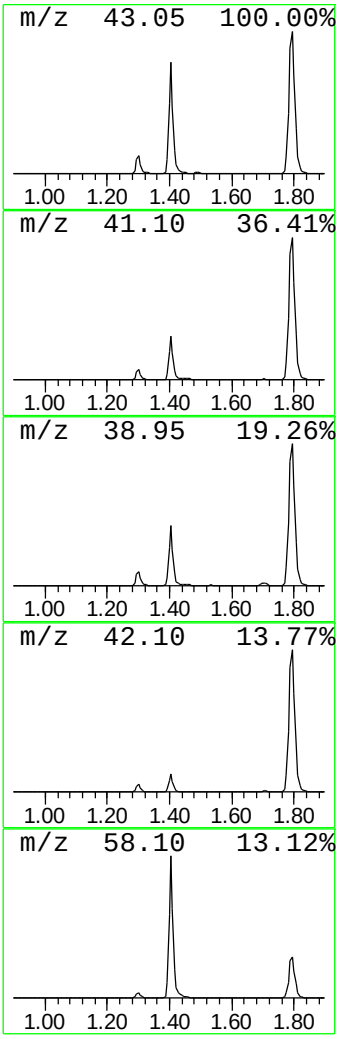
****

Peak Number 2 Butane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.40	127.28 ug/l	1156980	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	72
2	Propane, 2-nitro-	89	C3H7NO2	000079-46-9	9
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	9
4	Isobutane	58	C4H10	000075-28-5	9
5	Propane, 1-nitro-	89	C3H7NO2	000108-03-2	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

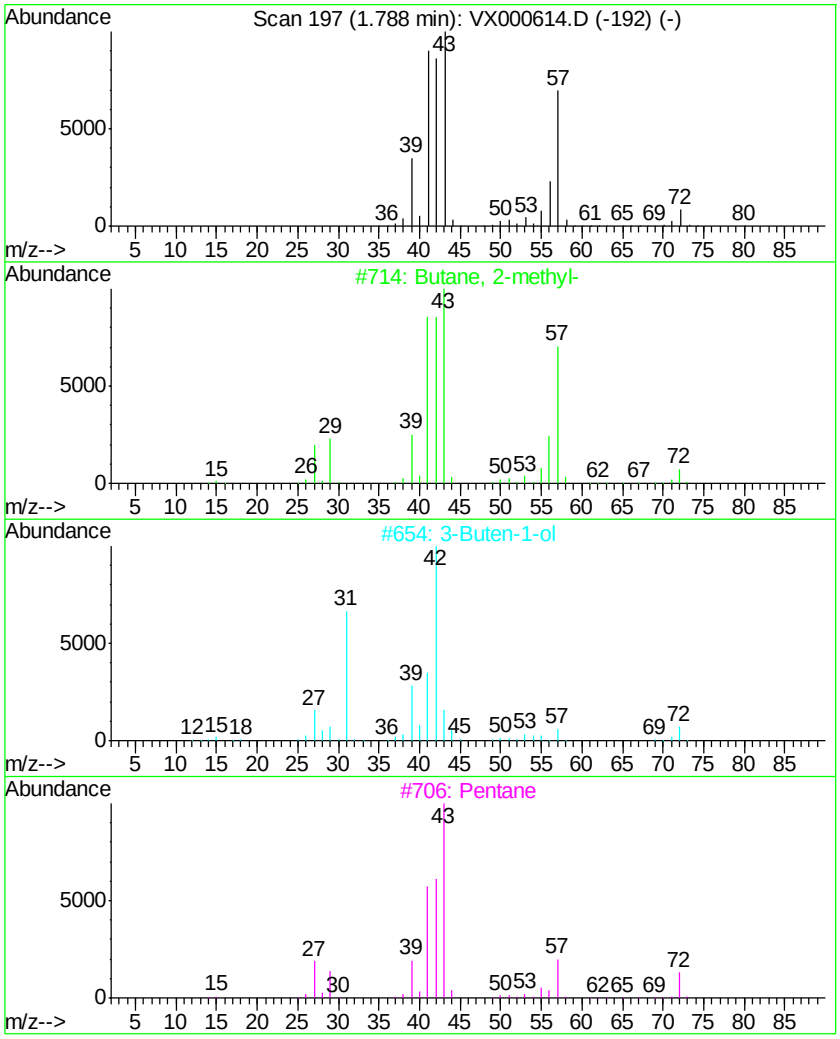
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

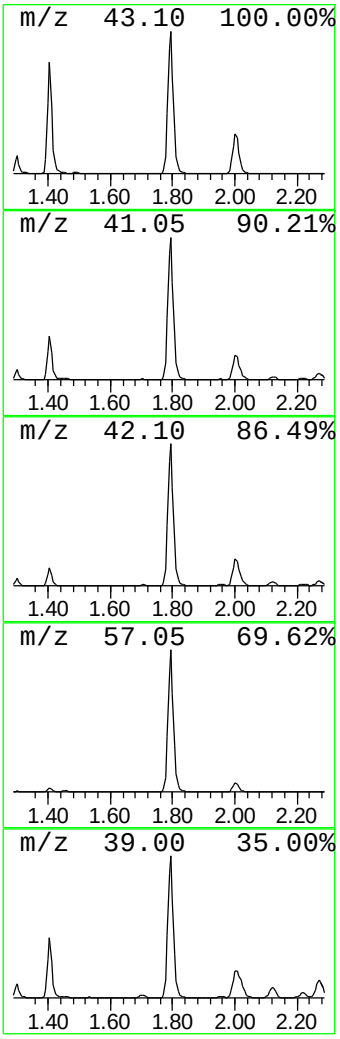
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.79	492.19 ug/l	4474040	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	33
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	10
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	10





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

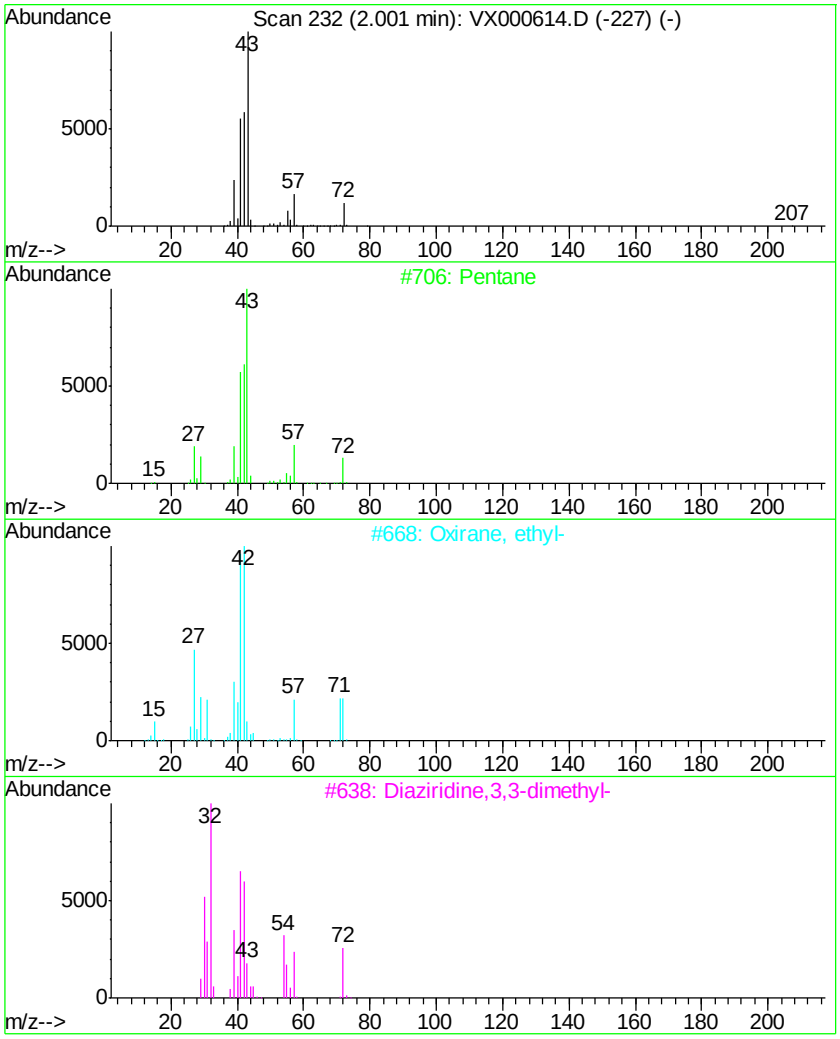
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

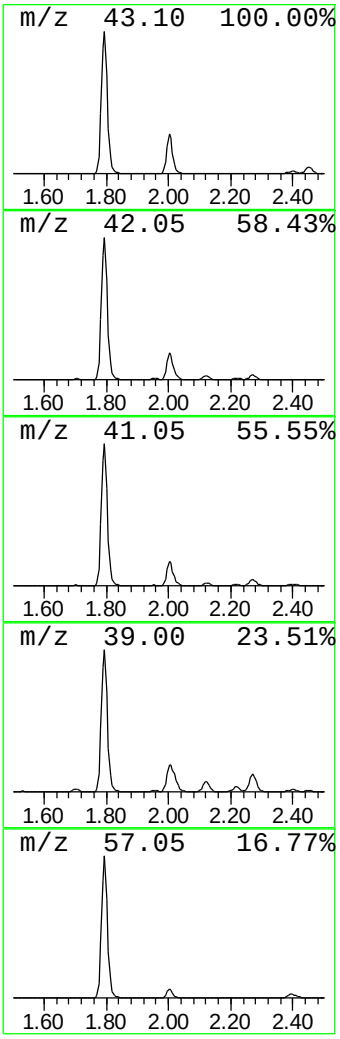
****

Peak Number 4 Pentane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.00	118.25 ug/l	1074870	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	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Butane, 2-methyl-	72	C5H12	000078-78-4	36
5	Tetrahydrofuran	72	C4H8O	000109-99-9	9





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

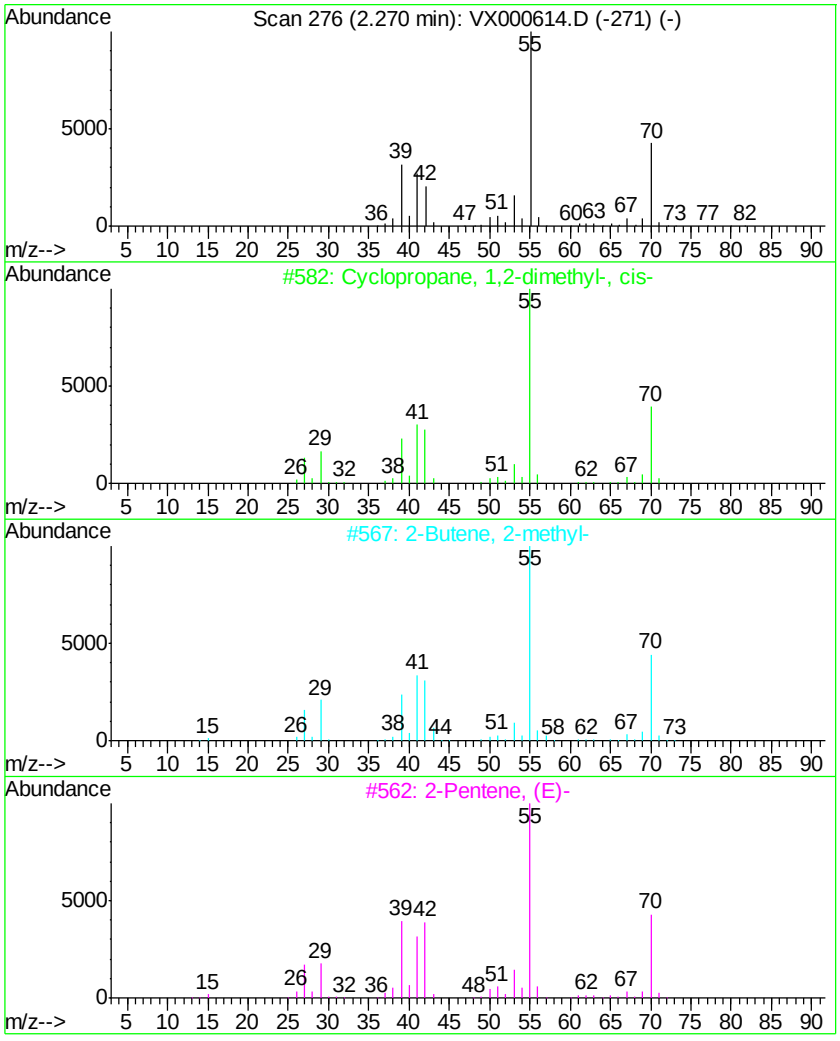
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

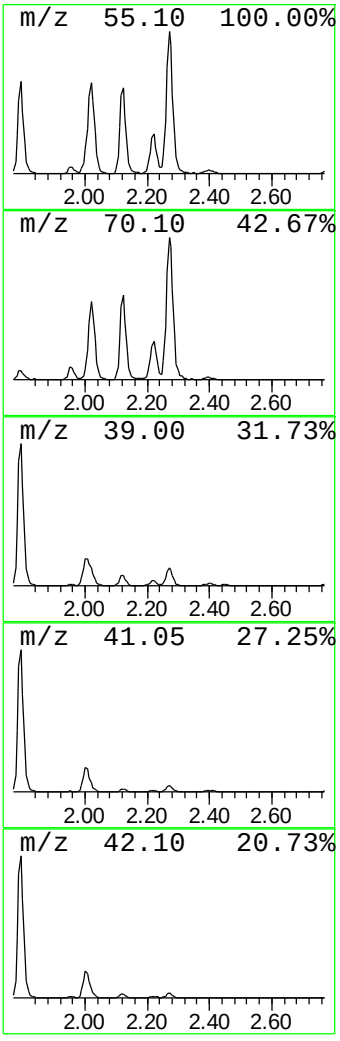
****

Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.27	50.44 ug/l	458461	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	90
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
3	2-Pentene, (E)-	70	C5H10	000646-04-8	86
4	Cyclopropane, 1,1-dimethyl-	70	C5H10	001630-94-0	80
5	2-Methyl-1-butene	70	C5H10	000563-46-2	72





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

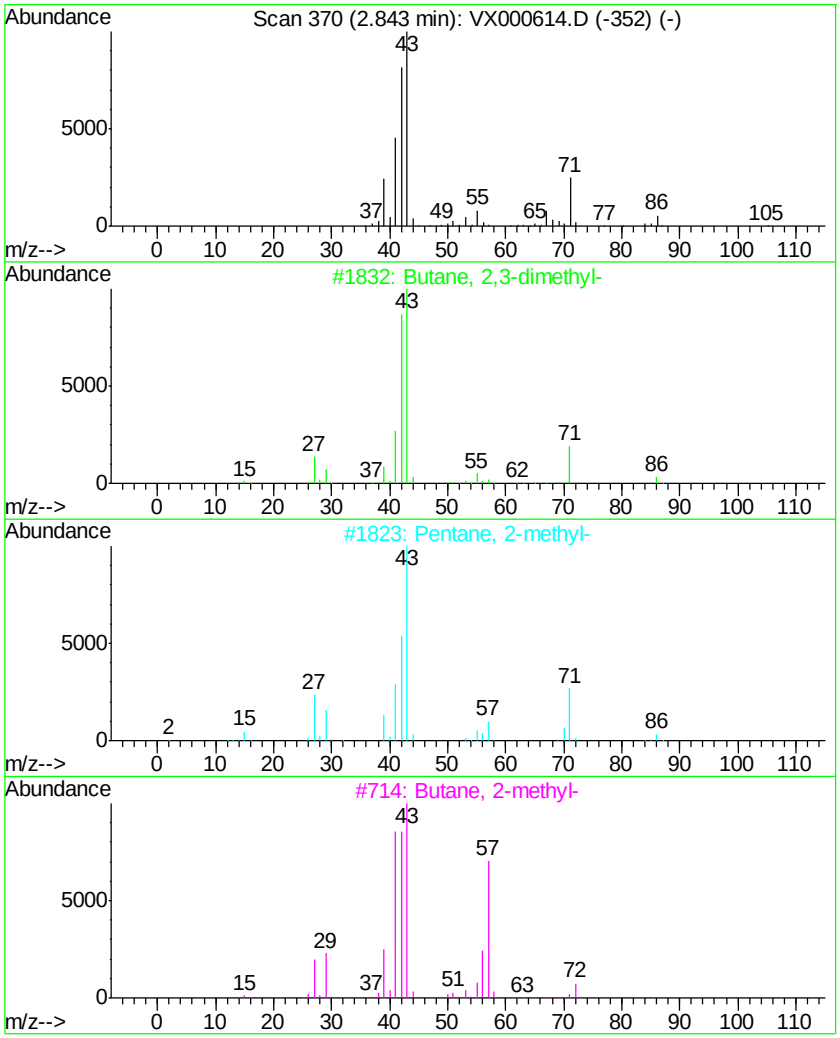
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

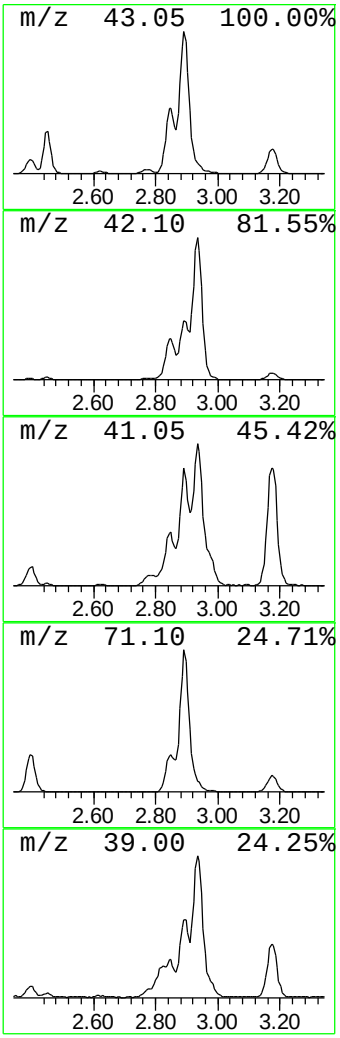
****

Peak Number 6 Butane, 2,3-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	62.54 ug/l	568508	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	86
2	Pentane, 2-methyl-	86	C6H14	000107-83-5	38
3	Butane, 2-methyl-	72	C5H12	000078-78-4	38
4	Tetrahydrofuran	72	C4H8O	000109-99-9	36
5	Pentane	72	C5H12	000109-66-0	36





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

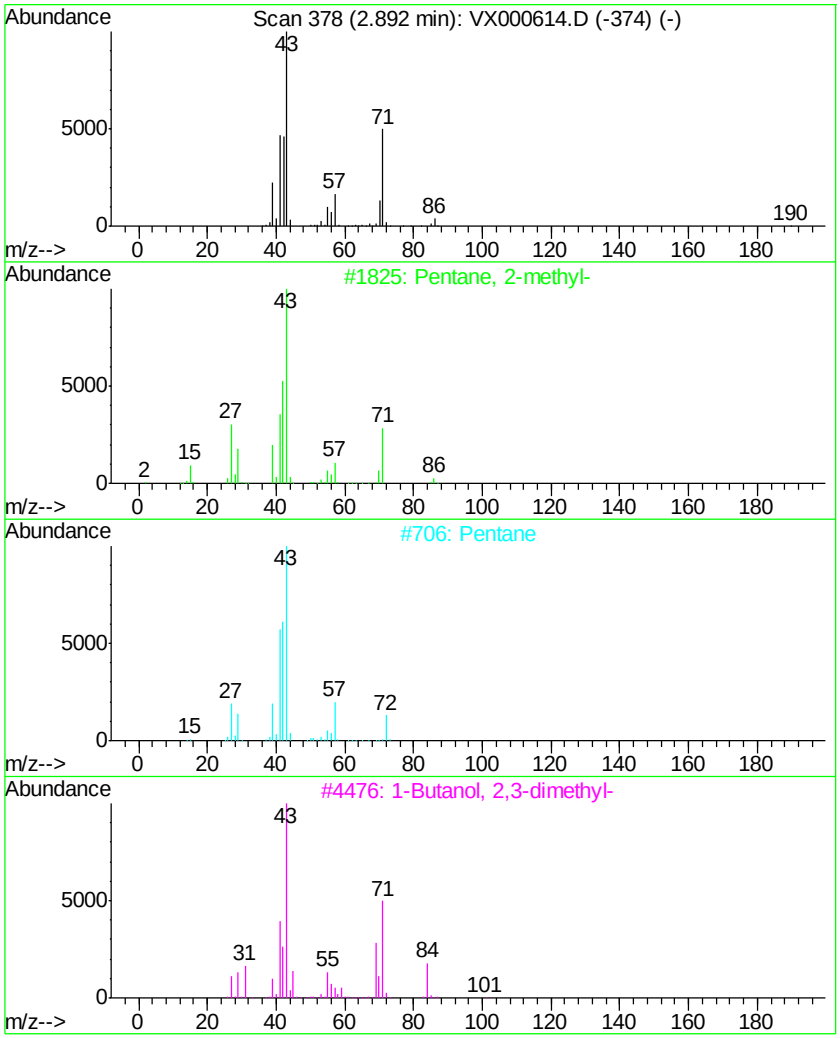
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

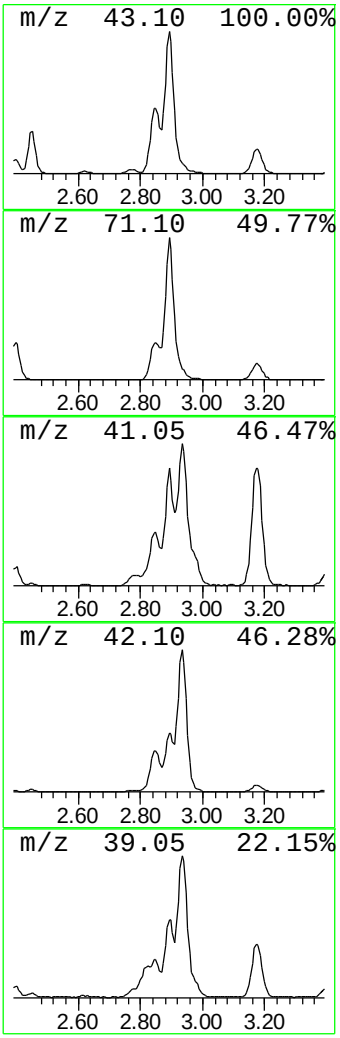
****

Peak Number 7 Pentane, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.89	76.57 ug/l	696023	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	72
2	Pentane	72	C5H12	000109-66-0	49
3	1-Butanol, 2,3-dimethyl-	102	C6H14O	019550-30-2	42
4	Hexane, 2,3-dimethyl-	114	C8H18	000584-94-1	38
5	Ether, hexyl pentyl	172	C11H24O	032357-83-8	33





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

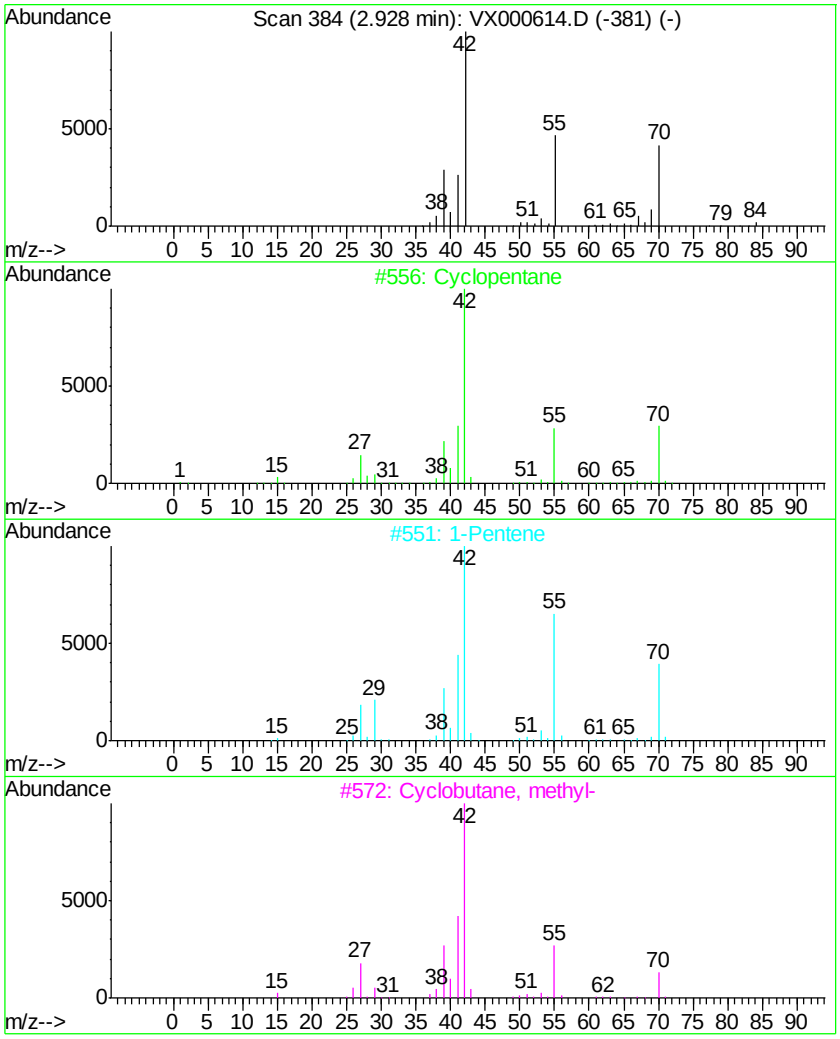
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

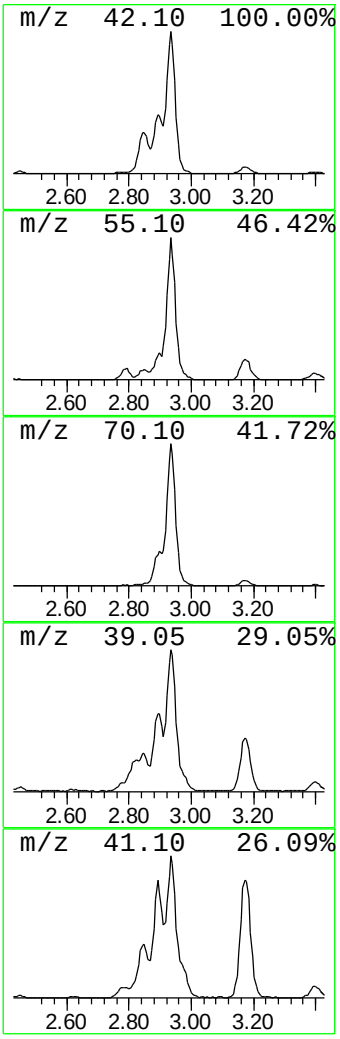
****

Peak Number 8 Cyclopentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.93	111.84 ug/l	1016650	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane	70	C5H10	000287-92-3	86
2	1-Pentene	70	C5H10	000109-67-1	80
3	Cyclobutane, methyl-	70	C5H10	000598-61-8	50
4	2H-Tetrazole, 2,5-dimethyl-	98	C3H6N4	004135-93-7	40
5	Cyclopropane, ethyl-	70	C5H10	001191-96-4	25





Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

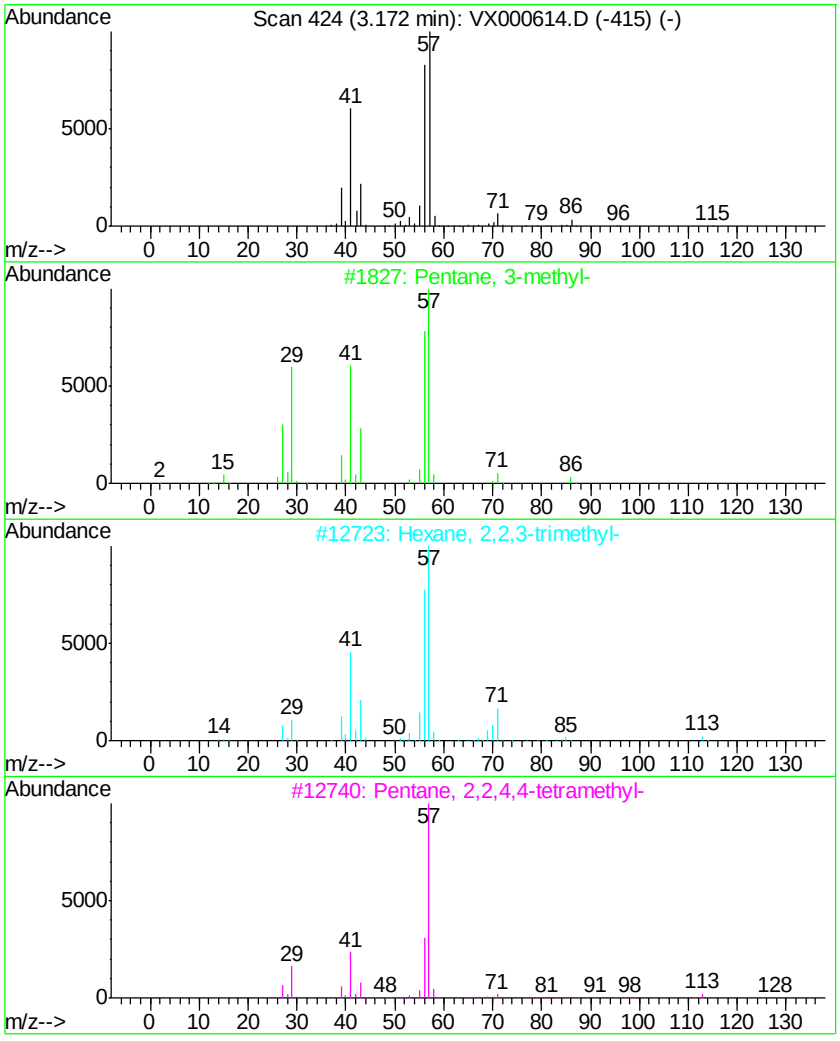
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

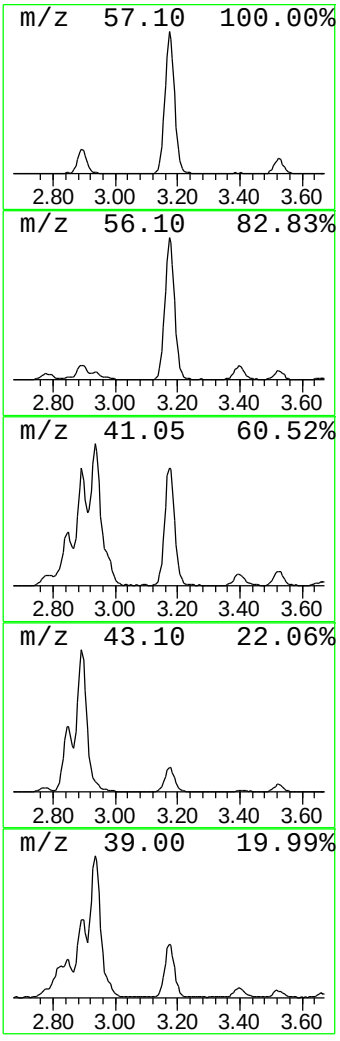
****

Peak Number 9 Pentane, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.17	71.27 ug/l	647868	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	Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45
4	Oxirane, (1-methylethyl)-	86	C5H10O	001438-14-8	45
5	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	43





Library Search Compound Report

Data Path : W:\HPCHEM1\MSVOA X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA X/WATER
ALS Vial : 35 Sample Multiplier: 1

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

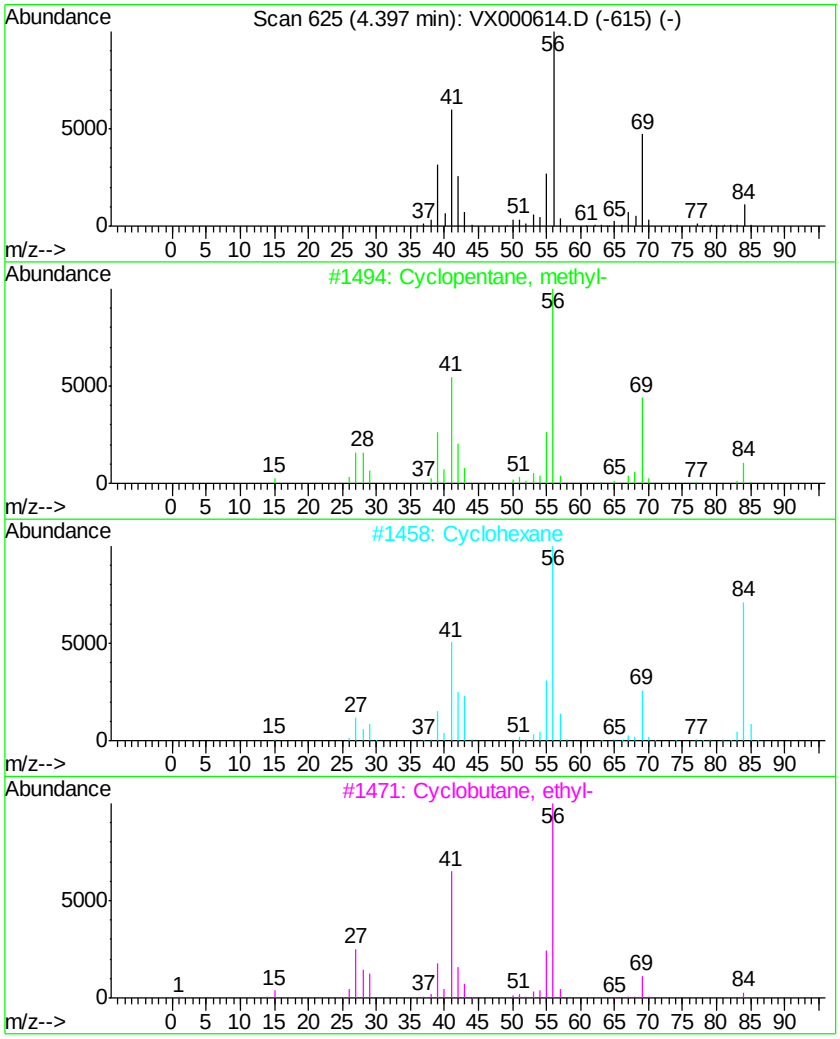
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

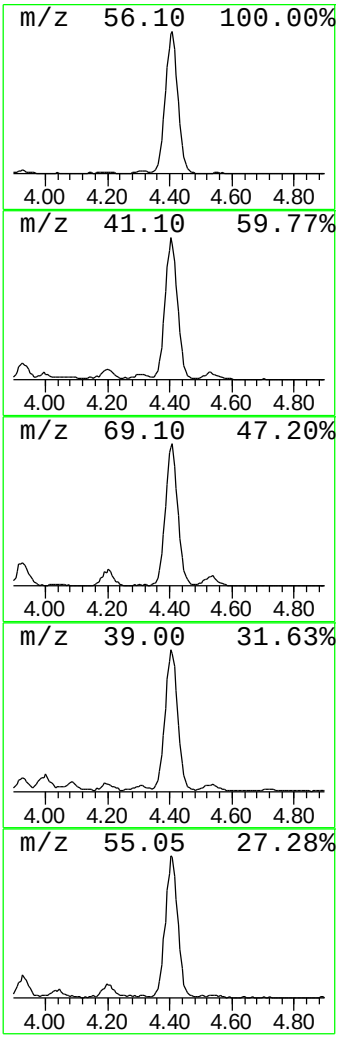
****

Peak Number 10 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.40	94.69 ug/l	860707	Pentafluorobenzene	5.68

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64
5	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_X\DATA\VX033118\
Data File : VX000614.D
Acq On : 01 Apr 2018 01:04
Operator : JC/MD
Sample : J2132-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 35 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	1.40	127.3	ug/l	1156980	1	5.68	454504	50.0
Butane, 2-methyl-	1.79	492.2	ug/l	4474040	1	5.68	454504	50.0
Pentane	2.00	118.3	ug/l	1074870	1	5.68	454504	50.0
Cyclopropane, 1,2...	2.27	50.4	ug/l	458461	1	5.68	454504	50.0
Butane, 2,3-dimet...	2.84	62.5	ug/l	568508	1	5.68	454504	50.0
Pentane, 2-methyl-	2.89	76.6	ug/l	696023	1	5.68	454504	50.0
Cyclopentane	2.93	111.8	ug/l	1016650	1	5.68	454504	50.0
Pentane, 3-methyl-	3.17	71.3	ug/l	647868	1	5.68	454504	50.0
Cyclopentane, met...	4.40	94.7	ug/l	860707	1	5.68	454504	50.0