LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072104.D
Acq On : 21 Apr 2022 02:42
Operator : JC\MD
Sample : N2482-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

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_N\methods\82N033022W.M
Title : SW846 8260

Signal : TIC: VN072104.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.134	184	195	216	rBV	5461702	12490370	7.94%	2.413%
2	3.510	250	259	279	rVB2	2085999	5551194	3.53%	1.072%
3	3.722	284	295	307	rBV	774531	1932594	1.23%	0.373%
4	3.998	333	342	356	rVB	1076006	2948202	1.87%	0.570%
5	5.157	531	539	553	rVV3	424346	2172406	1.38%	0.420%
6	5.616	600	617	637	rBV2	536332	1844777	1.17%	0.356%
7	6.469	755	762	774	rVB	797195	2428358	1.54%	0.469%
8	6.904	826	836	852	rVB	732953	2147524	1.37%	0.415%
9	7.145	864	877	886	rBV	2303228	6803265	4.33%	1.314%
10	8.086	1030	1037	1047	rVB2	1524016	3773493	2.40%	0.729%
11	8.457	1088	1100	1110	rBV	5875257	13788476	8.77%	2.664%
12	8.963	1176	1186	1200	rBV	1420263	3301012	2.10%	0.638%
13	10.439	1429	1437	1442	rBV	1818677	3474358	2.21%	0.671%
14	10.504	1442	1448	1464	rVB	8507116	15454634	9.83%	2.985%
15	11.739	1650	1658	1667	rBV	2035763	3582831	2.28%	0.692%
16	11.839	1667	1675	1685	rVV2	26287130	44224139	28.12%	8.543%
17	11.951	1685	1694	1713	rVB3	72099367	157269150	100.00%	30.381%
18	12.274	1738	1749	1769	rBV2	43852061	77688789	49.40%	15.008%
19	12.574	1789	1800	1809	rVB	1886412	3102559	1.97%	0.599%
20	12.727	1818	1826	1837	rVB	1624130	2719990	1.73%	0.525%
21	12.916	1851	1858	1863	rBV	3840770	6101154	3.88%	1.179%
22	12.980	1863	1869	1872	rVV	17427937	29669220	18.87%	5.731%
23	13.010	1872	1874	1878	rVV	7299249	9857248	6.27%	1.904%
24	13.057	1878	1882	1901	rVB	7683320	12156820	7.73%	2.348%
25	13.216	1901	1909	1923	rBV	9892723	16012108	10.18%	3.093%
26	13.363	1923	1934	1948	rBV	26602867	42535013	27.05%	8.217%
27	13.698	1980	1991	2007	rVB2	9578616	18505446	11.77%	3.575%
28	13.868	2015	2020	2037	rVB2	4570016	8962317	5.70%	1.731%
29	14.927	2191	2200	2206	rBV2	839082	1678360	1.07%	0.324%
30	15.498	2283	2297	2310	rBV	2949753	5485086	3.49%	1.060%

Sum of corrected areas: 517660893

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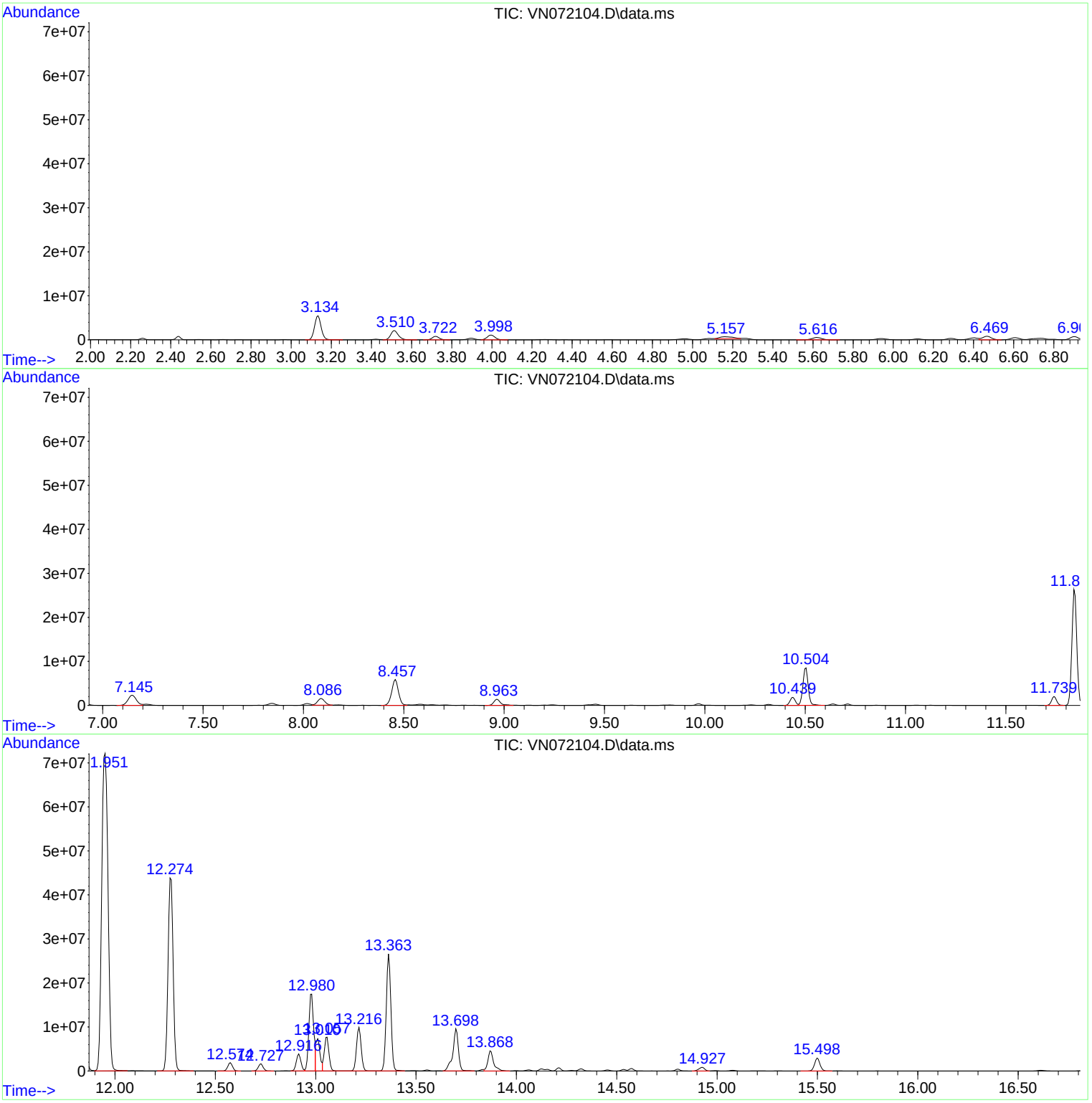
Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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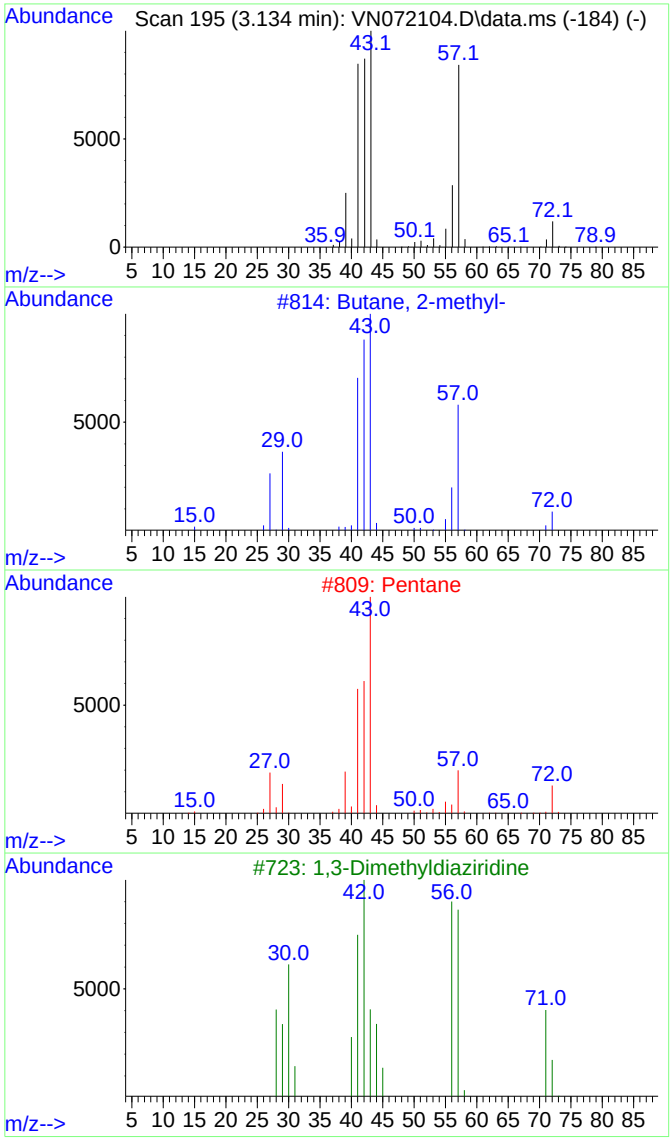
Quant Title : SW846 8260

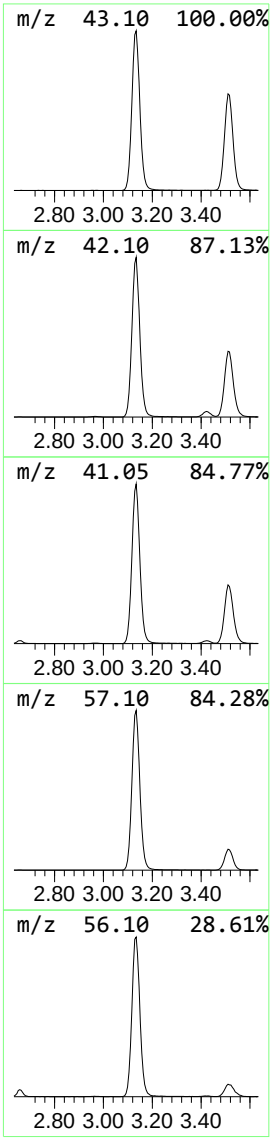
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.134	165.50 ug/l	12490400	Pentafluorobenzene	8.081

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	46
3	1,3-Dimethyldiaziridine	72	C3H8N2	026177-36-6	33
4	3-Buten-1-ol	72	C4H8O	000627-27-0	28
5	1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	12





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Data File : VN072104.D
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Operator : JC\MD
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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

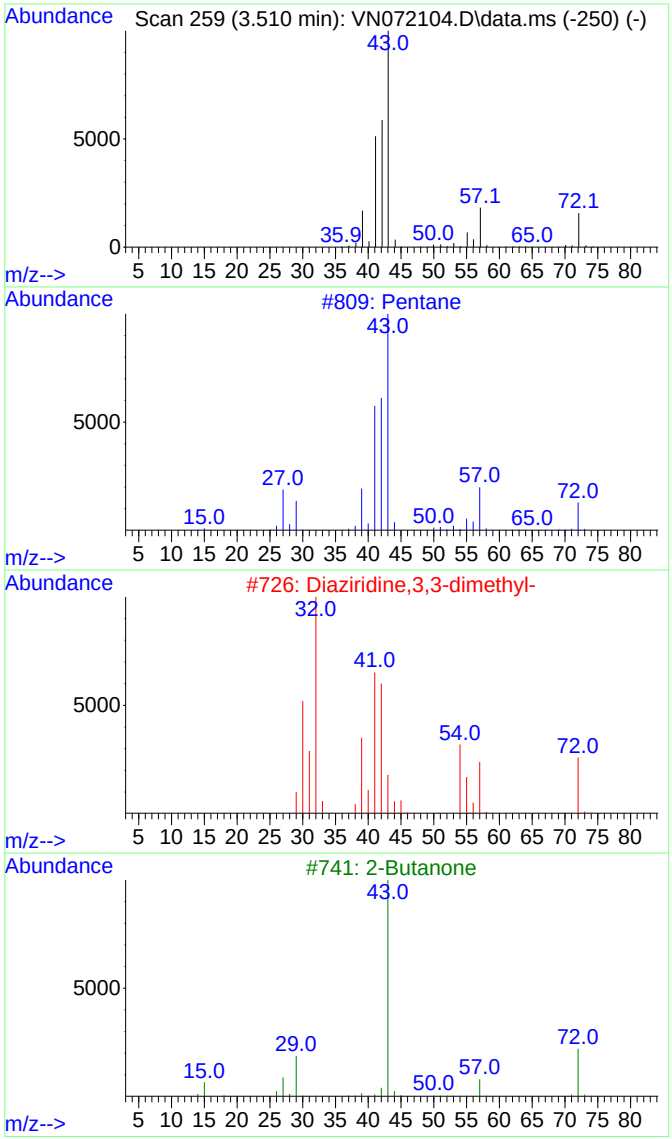
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

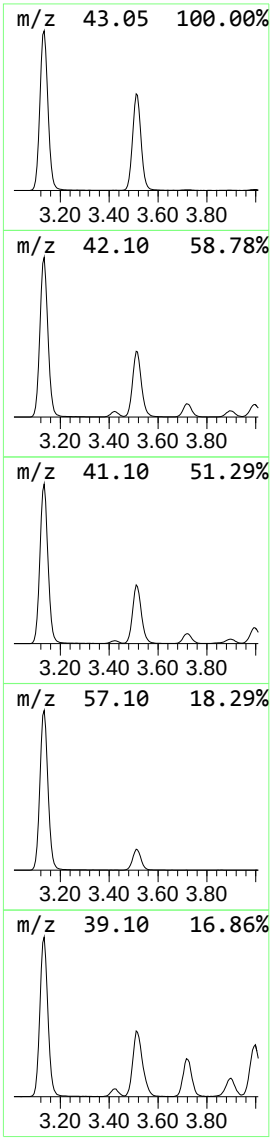
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Pentane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	73.56 ug/l	5551190	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	91
2	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
3	2-Butanone	72	C4H8O	000078-93-3	35
4	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	10
5	Butane, 2-methyl-	72	C5H12	000078-78-4	9





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Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

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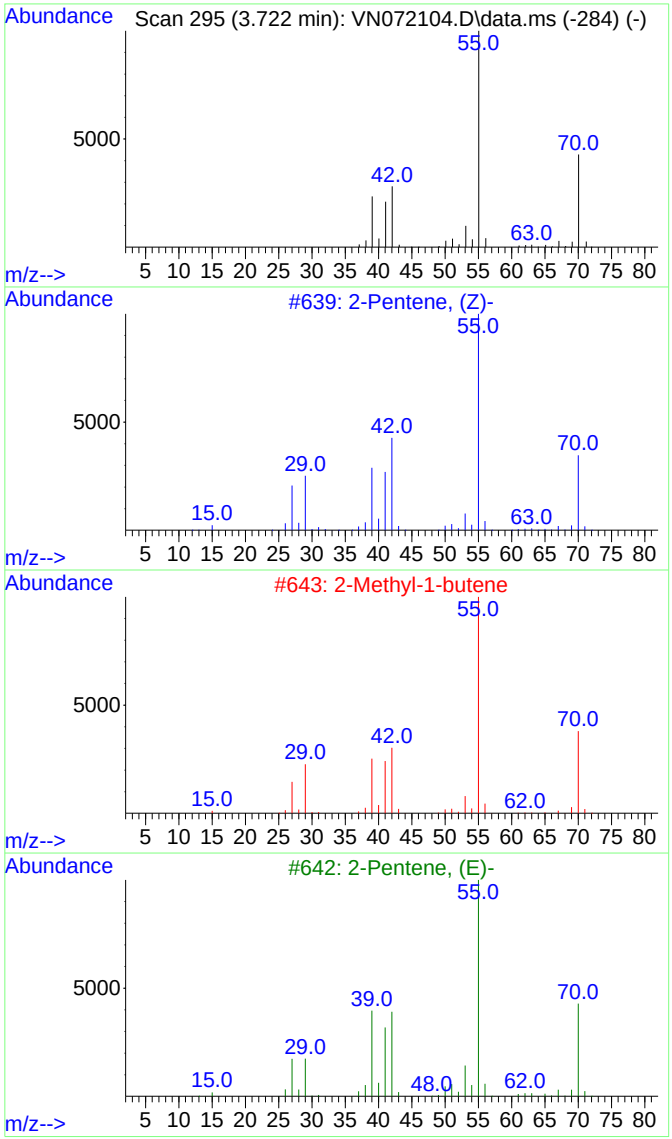
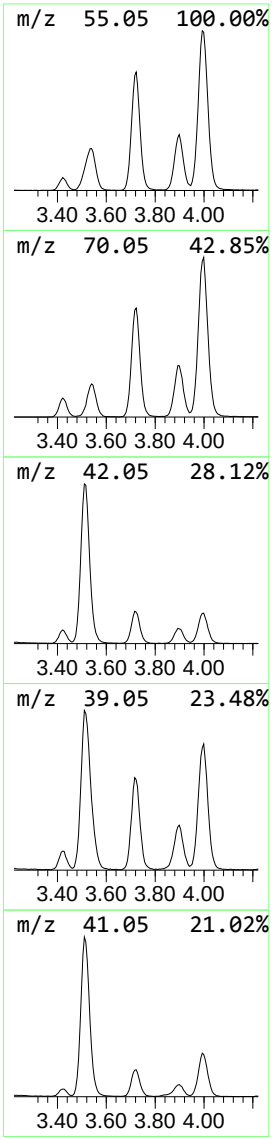
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentene, (Z)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.722	25.61 ug/l	1932590	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-	70	C5H10	000627-20-3	91
2	2-Methyl-1-butene	70	C5H10	000563-46-2	91
3	2-Pentene, (E)-	70	C5H10	000646-04-8	91
4	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
5	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91





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Instrument :
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ClientSampleId :
MW-14

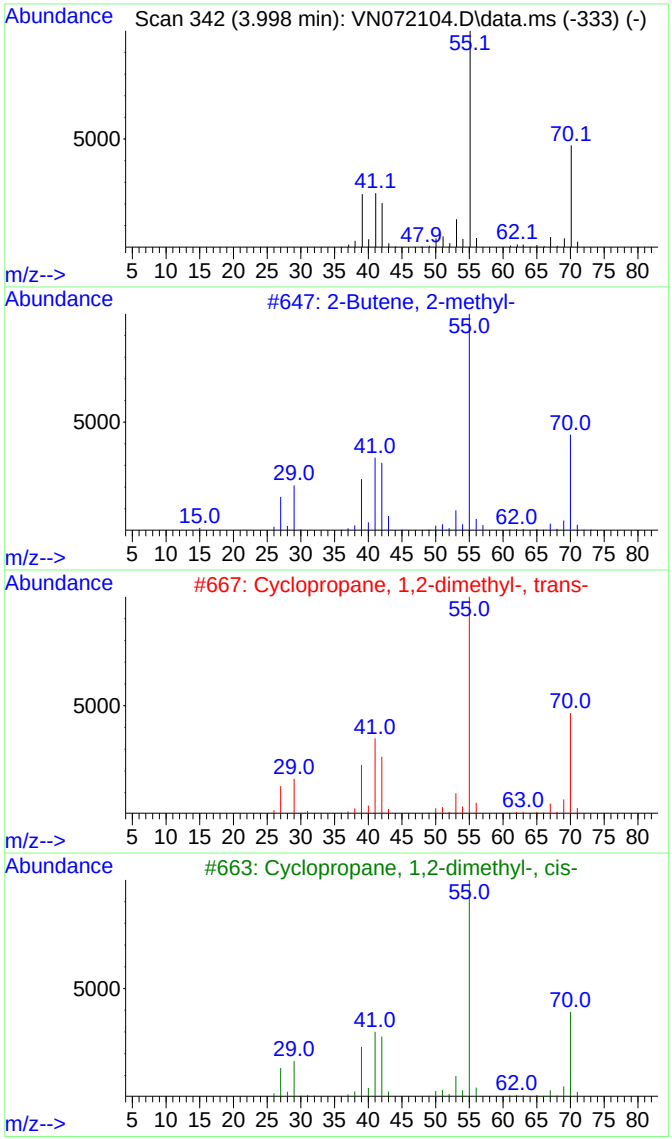
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

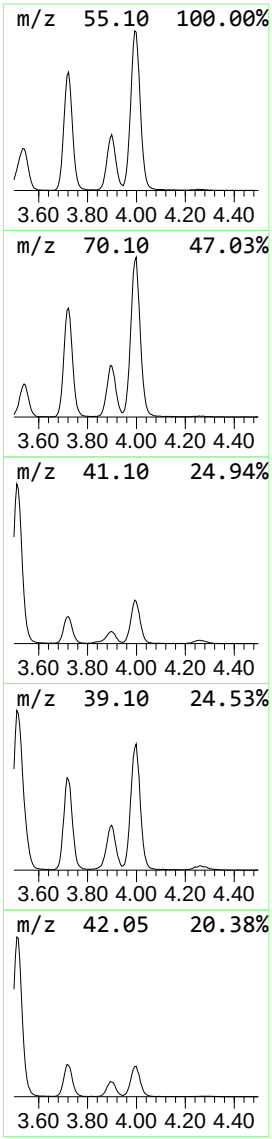
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 2-Butene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.998	39.06 ug/l	2948200	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	90
2	Cyclopropane, 1,2-dimethyl-, trans-	70	C5H10	002402-06-4	87
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	87
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5	2-Methyl-1-butene	70	C5H10	000563-46-2	83





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ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
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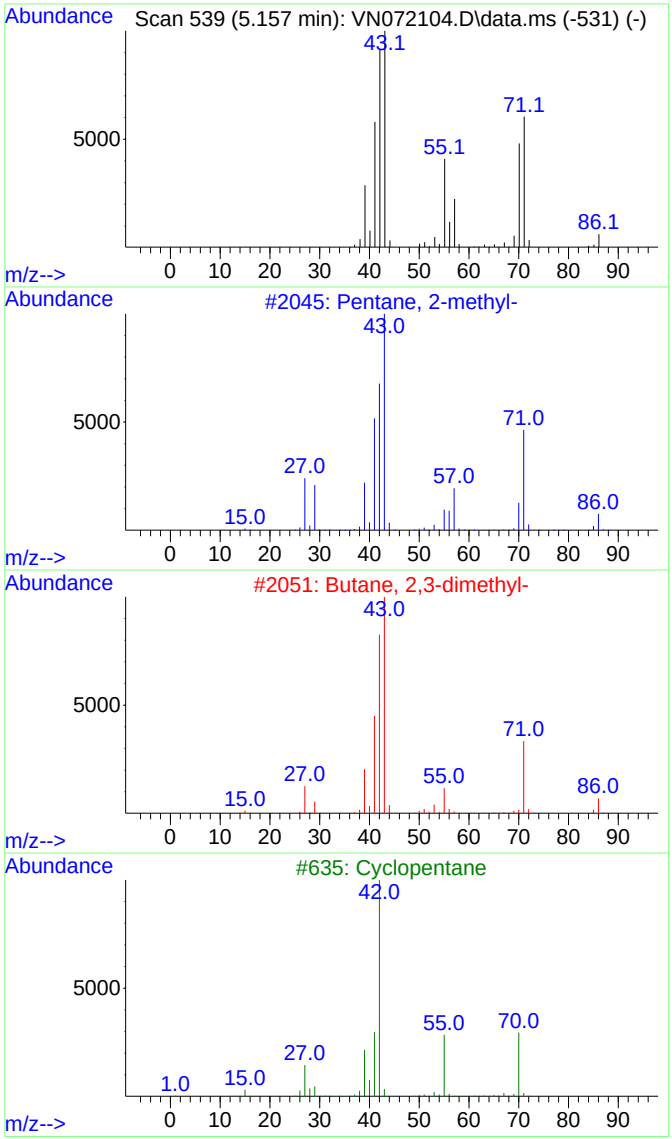
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

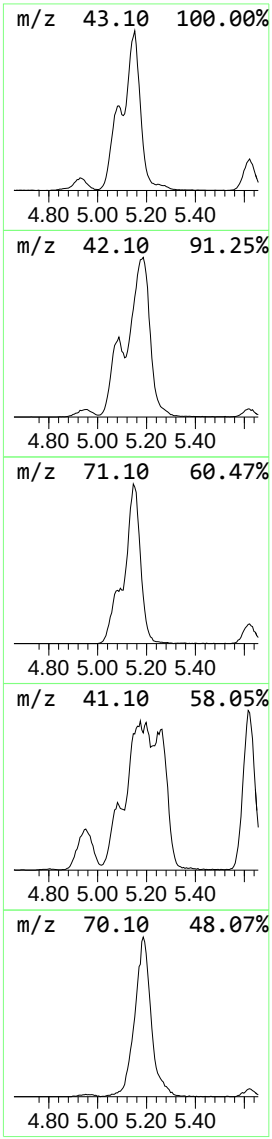
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.157	28.79 ug/l	2172410	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2-methyl-	86	C6H14	000107-83-5	53
2	Butane, 2,3-dimethyl-	86	C6H14	000079-29-8	50
3	Cyclopentane	70	C5H10	000287-92-3	49
4	1-Pentene	70	C5H10	000109-67-1	47
5	Heptane, 4-methyl-	114	C8H18	000589-53-7	43





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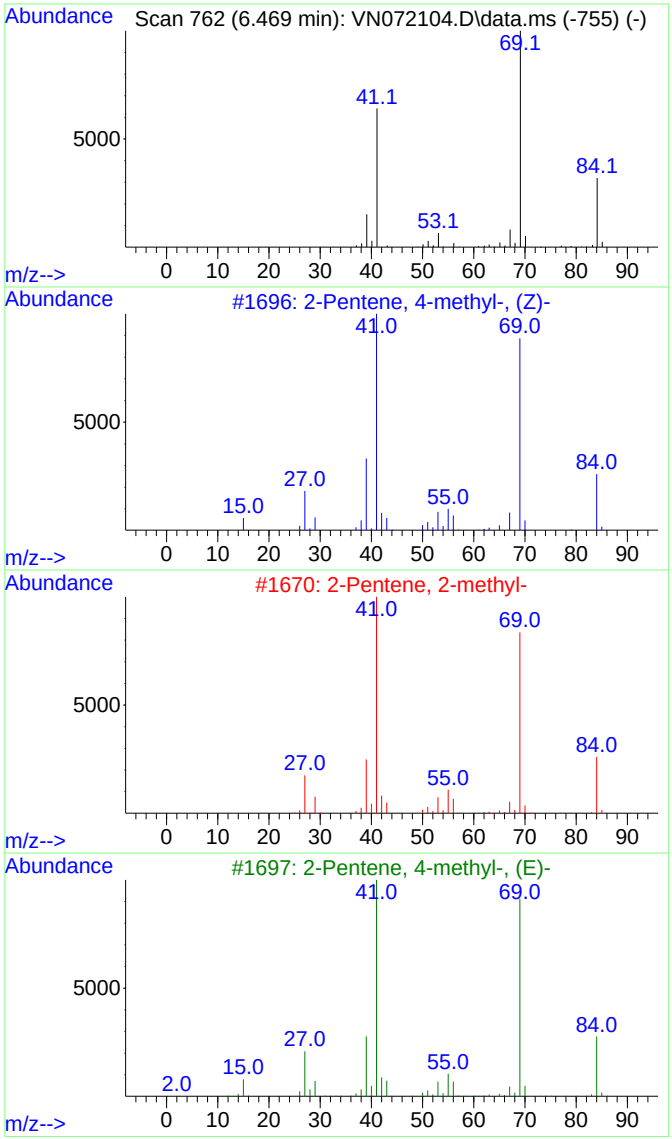
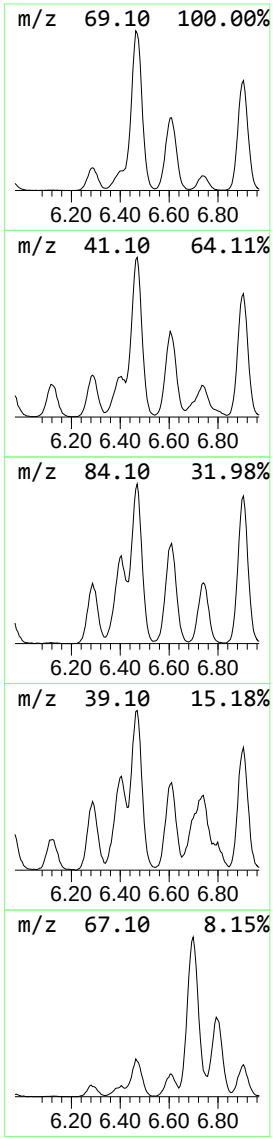
****
Peak Number 6 2-Pentene, 4-methyl-, (Z)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.469	32.18 ug/l	2428360	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	90
2	2-Pentene, 2-methyl-	84	C6H12	000625-27-4	90
3	2-Pentene, 4-methyl-, (E)-	84	C6H12	000674-76-0	90
4	Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	83
5	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	83





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TIC Library : C:\Database\NIST20.L
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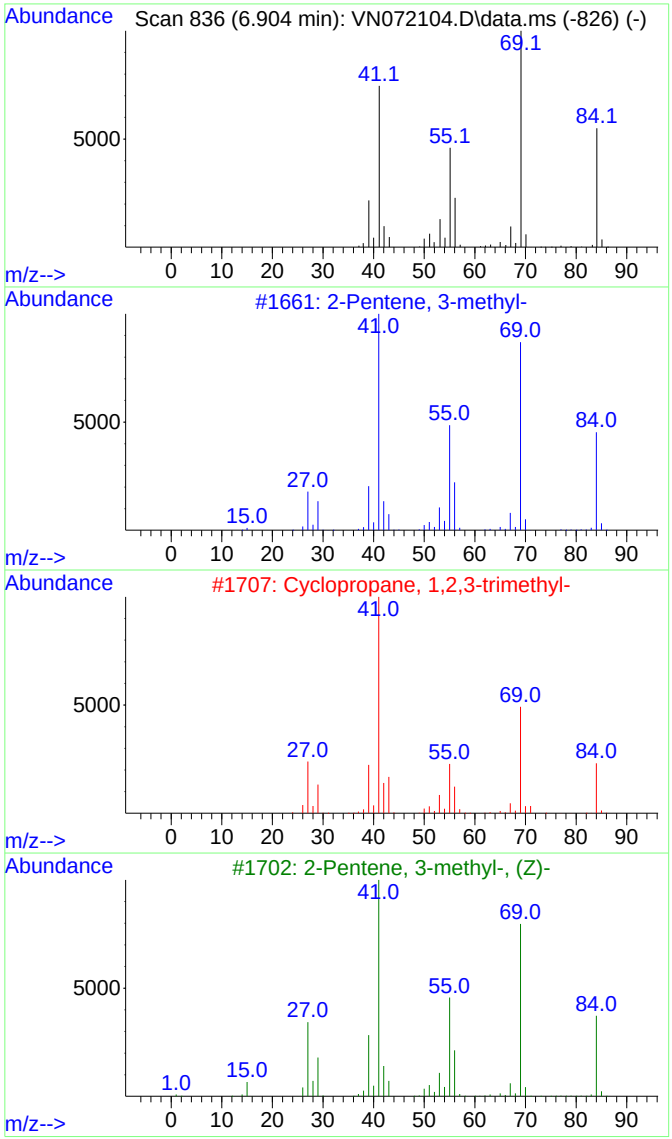
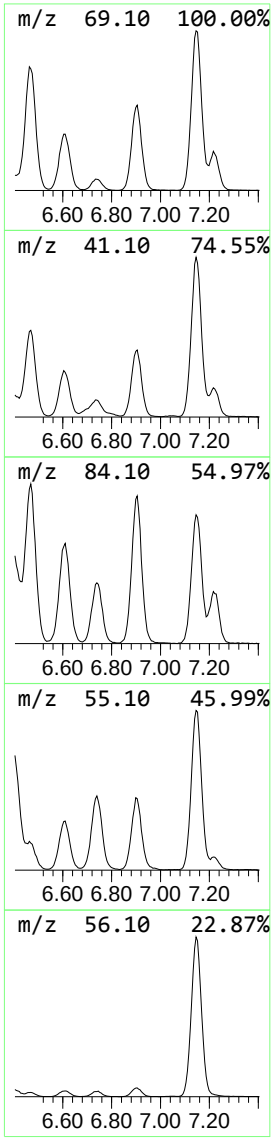
****

Peak Number 7 2-Pentene, 3-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.904	28.46 ug/l	2147520	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 3-methyl-	84	C6H12	000922-61-2	91
2	Cyclopropane, 1,2,3-trimethyl-	84	C6H12	042984-19-0	91
3	2-Pentene, 3-methyl-, (Z)-	84	C6H12	000922-62-3	91
4	2-Pentene, 3-methyl-, (E)-	84	C6H12	000616-12-6	91
5	Cyclopropane, 1,1,2-trimethyl-	84	C6H12	004127-45-1	86





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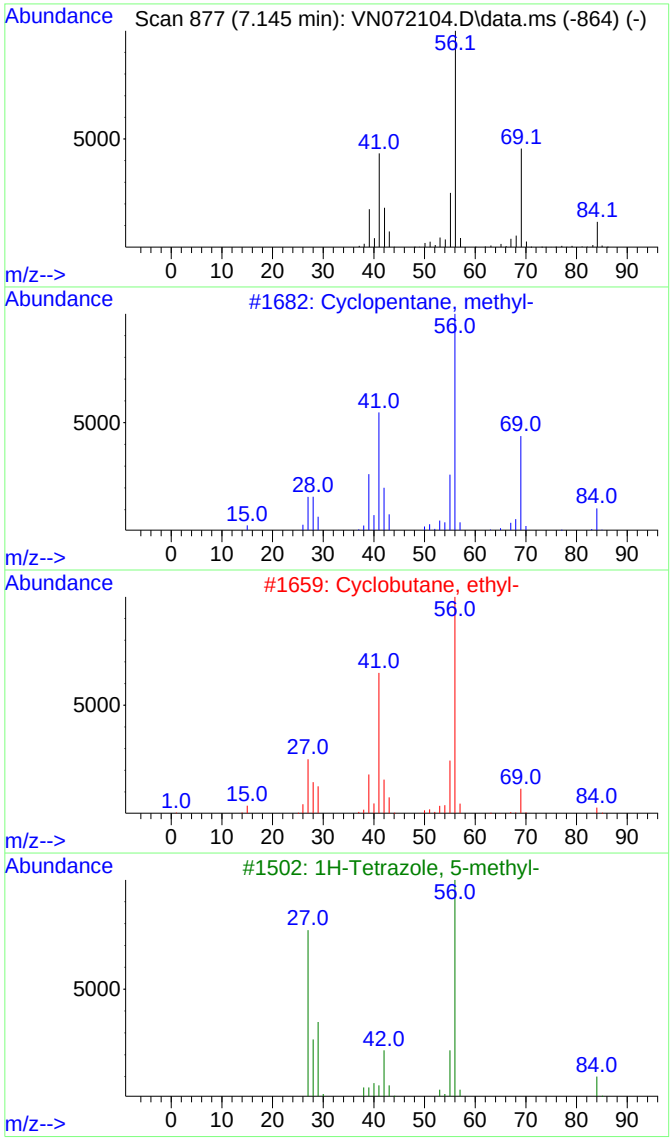
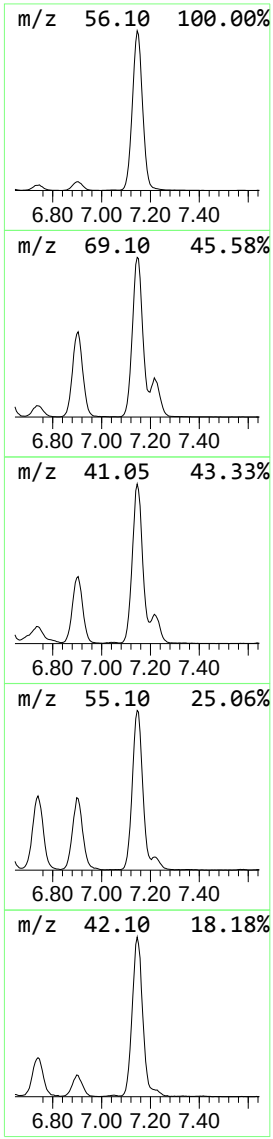
****
Peak Number 8 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	90.15 ug/l	6803270	Pentafluorobenzene	8.081

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	78
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
4	Cyclohexane	84	C6H12	000110-82-7	56
5	1-Hexene	84	C6H12	000592-41-6	52





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Instrument :
MSVOA_N
ClientSampleId :
MW-14

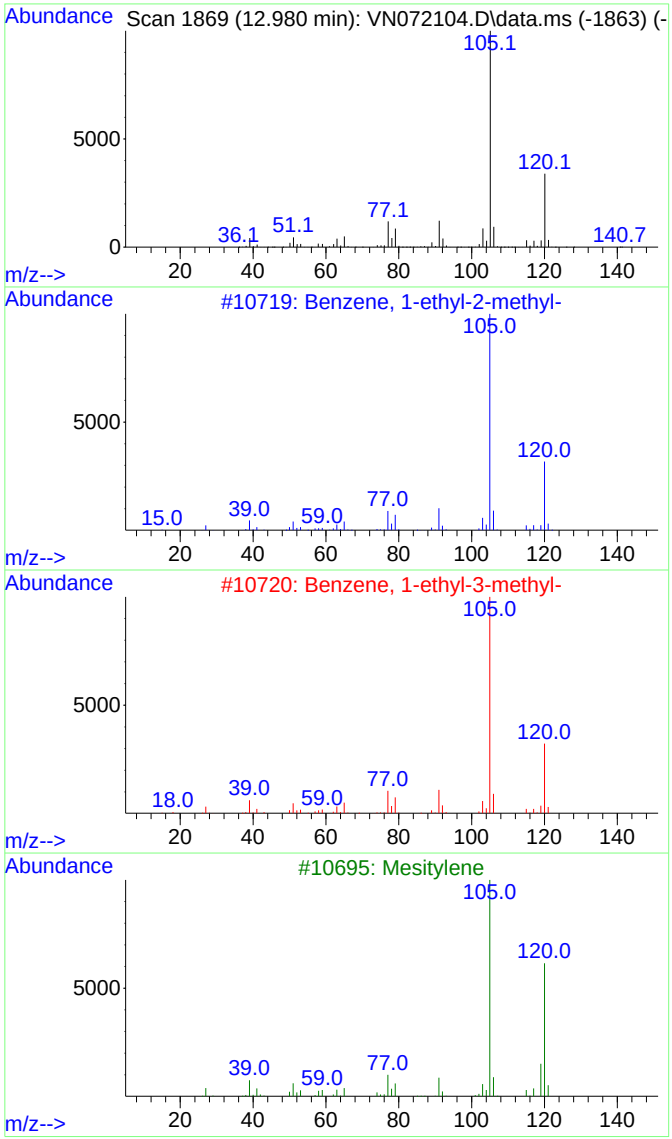
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

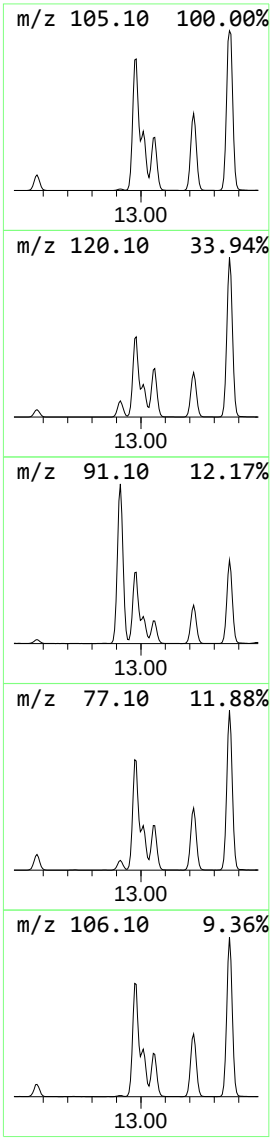
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	80.16 ug/l	29669200	1,4-Dichlorobenzene-d4	13.668

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	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





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ClientSampleId :
MW-14

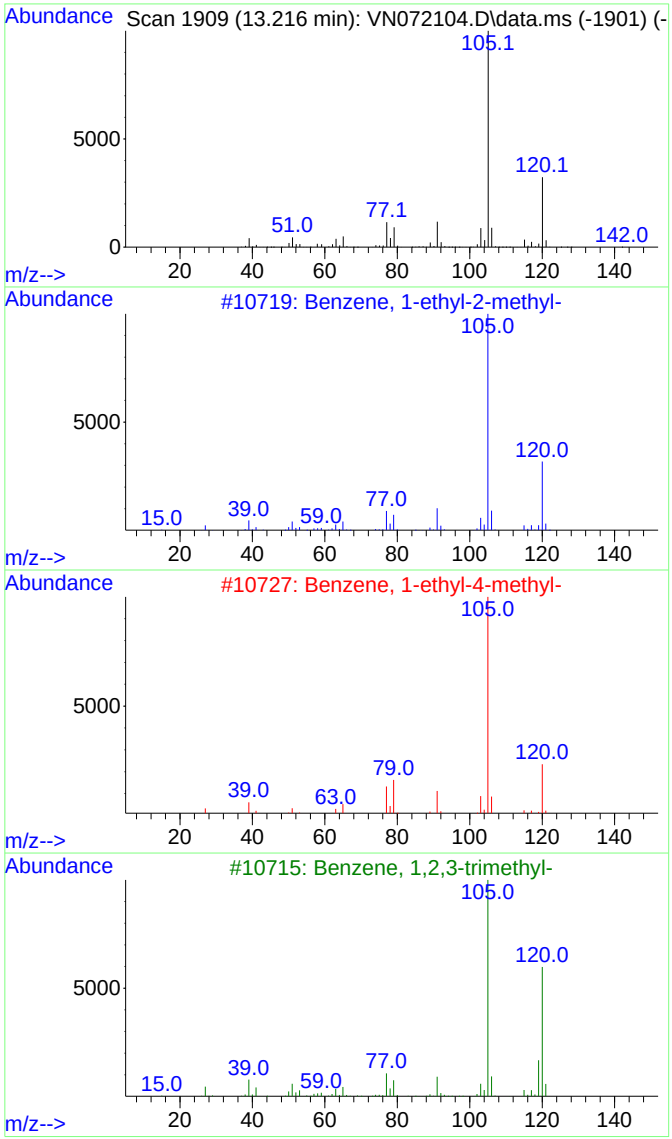
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

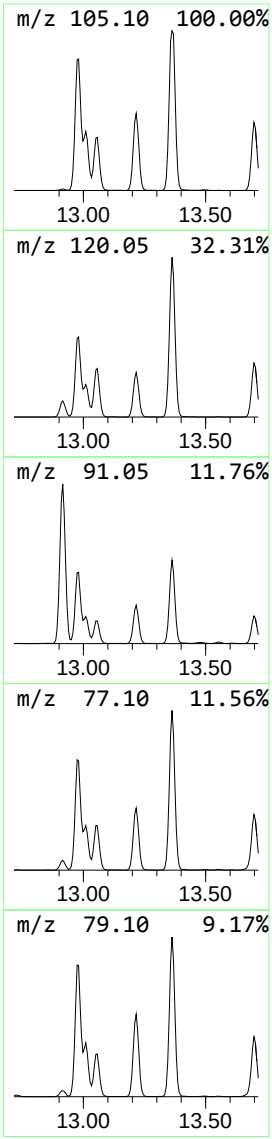
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	43.26 ug/l	16012100	1,4-Dichlorobenzene-d4	13.668

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-4-methyl-	120	C9H12	000622-96-8	94
3	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5	Mesitylene	120	C9H12	000108-67-8	91





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042022\
Data File : VN072104.D
Acq On : 21 Apr 2022 02:42
Operator : JC\MD
Sample : N2482-09
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N033022W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-methyl-	3.134	165.5	ug/l	12490400	1	8.081	3773490	50.0
Pentane	3.510	73.6	ug/l	5551190	1	8.081	3773490	50.0
2-Pentene, (Z)-	3.722	25.6	ug/l	1932590	1	8.081	3773490	50.0
2-Butene, 2-met...	3.998	39.1	ug/l	2948200	1	8.081	3773490	50.0
Pentane, 2-methyl-	5.157	28.8	ug/l	2172410	1	8.081	3773490	50.0
2-Pentene, 4-me...	6.469	32.2	ug/l	2428360	1	8.081	3773490	50.0
2-Pentene, 3-me...	6.904	28.5	ug/l	2147520	1	8.081	3773490	50.0
Cyclopentane, m...	7.145	90.2	ug/l	6803270	1	8.081	3773490	50.0
Benzene, 1-ethy...	12.980	80.2	ug/l	29669200	4	13.668	18505400	50.0
Benzene, 1-ethy...	13.216	43.3	ug/l	16012100	4	13.668	18505400	50.0