LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N042622W.M
Title : SW846 8260

Signal : TIC: VN072249.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.257	36	46	60	rBV3	132352	416473	23.93%	2.582%
2	2.440	71	77	86	rVB	135143	214620	12.33%	1.331%
3	2.963	160	166	175	rVB3	9807	22657	1.30%	0.140%
4	3.128	184	194	206	rVB	166152	392420	22.54%	2.433%
5	3.340	221	230	236	rBV	22192	54557	3.13%	0.338%
6	3.422	238	244	251	rVV	24331	52758	3.03%	0.327%
7	3.522	251	261	278	rVB5	62845	218487	12.55%	1.355%
8	3.722	285	295	307	rBV	66643	168487	9.68%	1.045%
9	3.898	312	325	332	rBV2	45309	121291	6.97%	0.752%
10	3.998	332	342	353	rVB	72643	198572	11.41%	1.231%
11	4.187	364	374	382	rBV3	11064	30750	1.77%	0.191%
12	4.963	495	506	516	rBV4	18348	63257	3.63%	0.392%
13	5.098	519	529	530	rVV6	9085	25840	1.48%	0.160%
14	5.187	533	544	567	rVB5	37079	183078	10.52%	1.135%
15	5.616	604	617	629	rBV4	13748	44413	2.55%	0.275%
16	5.939	664	672	685	rVB6	8048	29843	1.71%	0.185%
17	6.387	739	748	757	rBV6	9735	34200	1.96%	0.212%
18	6.475	757	763	772	rVB4	7974	22410	1.29%	0.139%
19	6.604	775	785	793	rBV4	10710	29744	1.71%	0.184%
20	6.704	793	802	808	rBV4	11237	35707	2.05%	0.221%
21	6.904	827	836	847	rVB4	9130	25703	1.48%	0.159%
22	7.145	863	877	887	rBV5	47405	146473	8.41%	0.908%
23	7.328	896	908	918	rBV3	40585	110352	6.34%	0.684%
24	7.833	984	994	1007	rVB5	14886	47199	2.71%	0.293%
25	8.016	1015	1025	1030	rBV	207138	491306	28.23%	3.047%
26	8.081	1030	1036	1048	rVB	388115	902088	51.83%	5.594%
27	8.439	1086	1097	1109	rBV2	280921	836997	48.09%	5.190%
28	8.586	1116	1122	1128	rBV6	12892	25404	1.46%	0.158%
29	8.963	1178	1186	1203	rBV	605956	1242168	71.36%	7.702%
30	9.216	1221	1229	1239	rVB	114664	237634	13.65%	1.474%
31	10.439	1426	1437	1443	rBV	945495	1740619	100.00%	10.793%
32	10.504	1443	1448	1462	rVV	194058	374487	21.51%	2.322%
33	10.639	1466	1471	1477	rVV2	15013	26798	1.54%	0.166%
34	10.716	1477	1484	1489	rVB3	12803	23559	1.35%	0.146%
35	10.974	1519	1528	1536	rBV3	25683	43882	2.52%	0.272%
36	11.739	1648	1658	1669	rBV	978049	1733048	99.57%	10.746%

LSC Area Percent Report

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

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\82N042622W.M
Title : SW846 8260

37	11.839	1669	1675	1686	rVV	343889	594611	34.16%	3.687%
38	11.951	1686	1694	1705	rVB	430269	864454	49.66%	5.360%
39	12.274	1741	1749	1762	rVB	460404	784852	45.09%	4.867%
40	12.574	1794	1800	1806	rBV3	11609	19307	1.11%	0.120%
41	12.727	1816	1826	1838	rBV	756632	1293782	74.33%	8.023%
42	12.915	1853	1858	1863	rBV	24840	38637	2.22%	0.240%
43	12.980	1863	1869	1872	rVV	39068	68767	3.95%	0.426%
44	13.010	1872	1874	1878	rVV2	31019	43426	2.49%	0.269%
45	13.051	1878	1881	1891	rVB2	27763	44333	2.55%	0.275%
46	13.215	1902	1909	1918	rBV	60304	101985	5.86%	0.632%
47	13.363	1927	1934	1945	rBV	121460	202071	11.61%	1.253%
48	13.668	1978	1986	2000	rBV	792033	1474949	84.74%	9.146%
49	13.874	2015	2021	2030	rVB2	42797	77658	4.46%	0.482%
50	14.927	2192	2200	2205	rBV4	12256	25755	1.48%	0.160%
51	15.509	2286	2299	2308	rBV	54882	124975	7.18%	0.775%

Sum of corrected areas: 16126843

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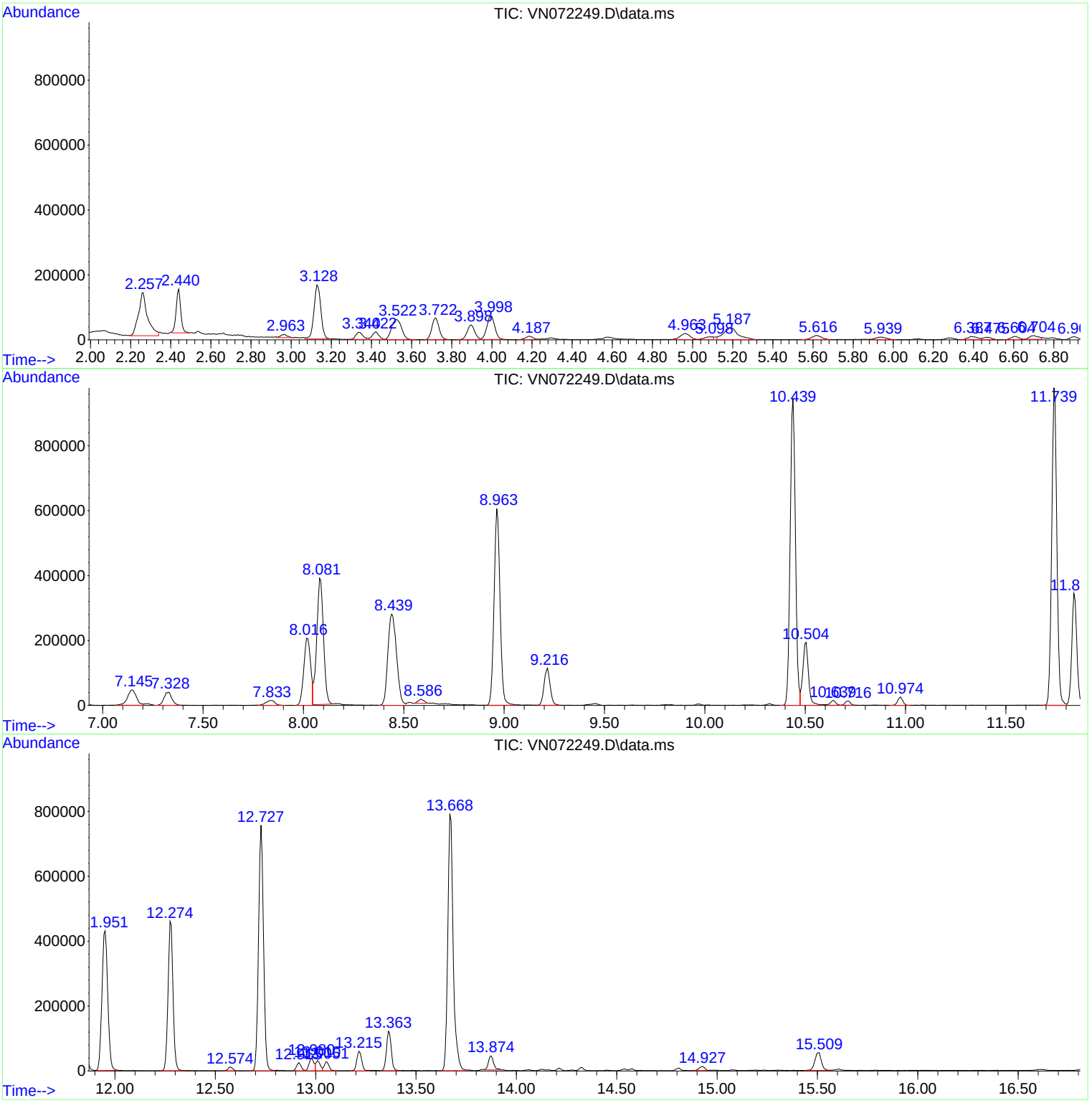
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
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ClientSampleId :
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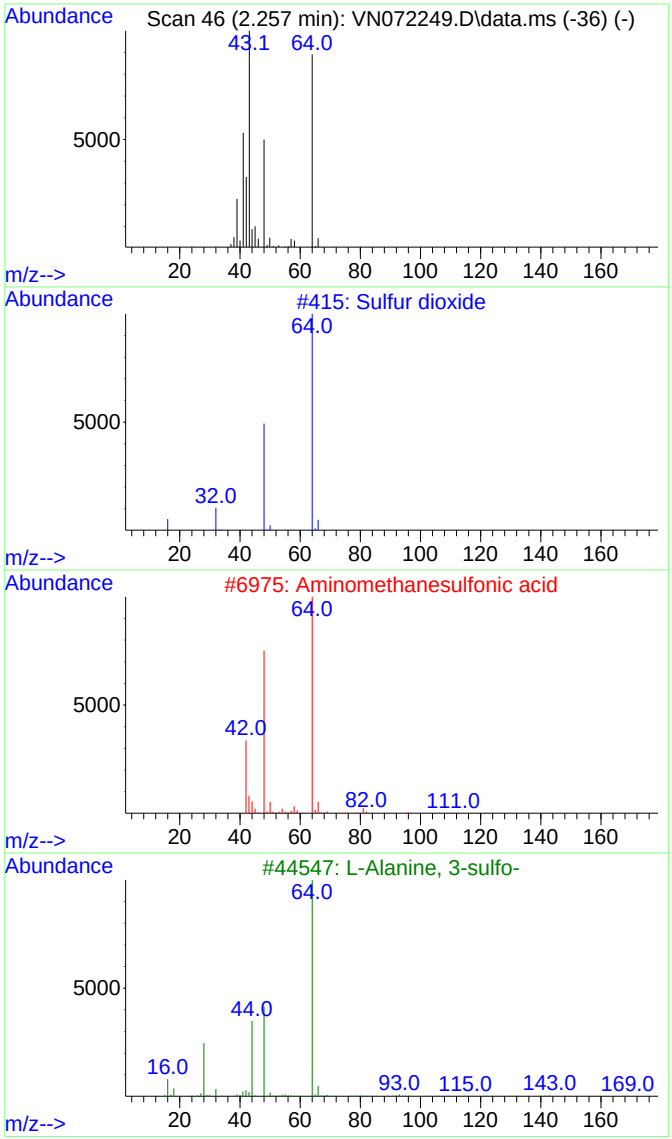
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

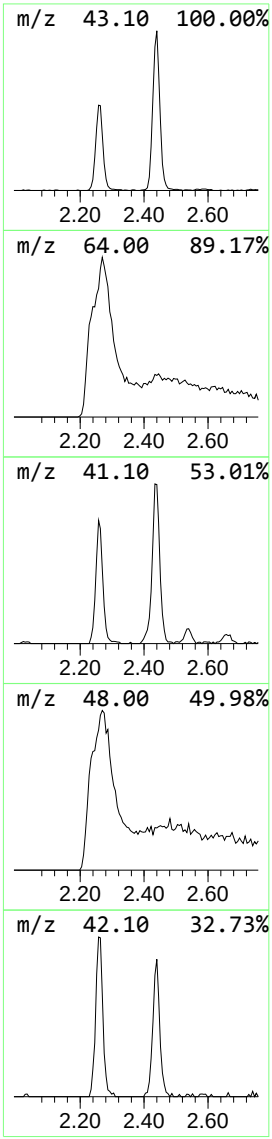
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.257	23.08 ug/l	416473	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	80
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	4





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Data File : VN072249.D
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Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

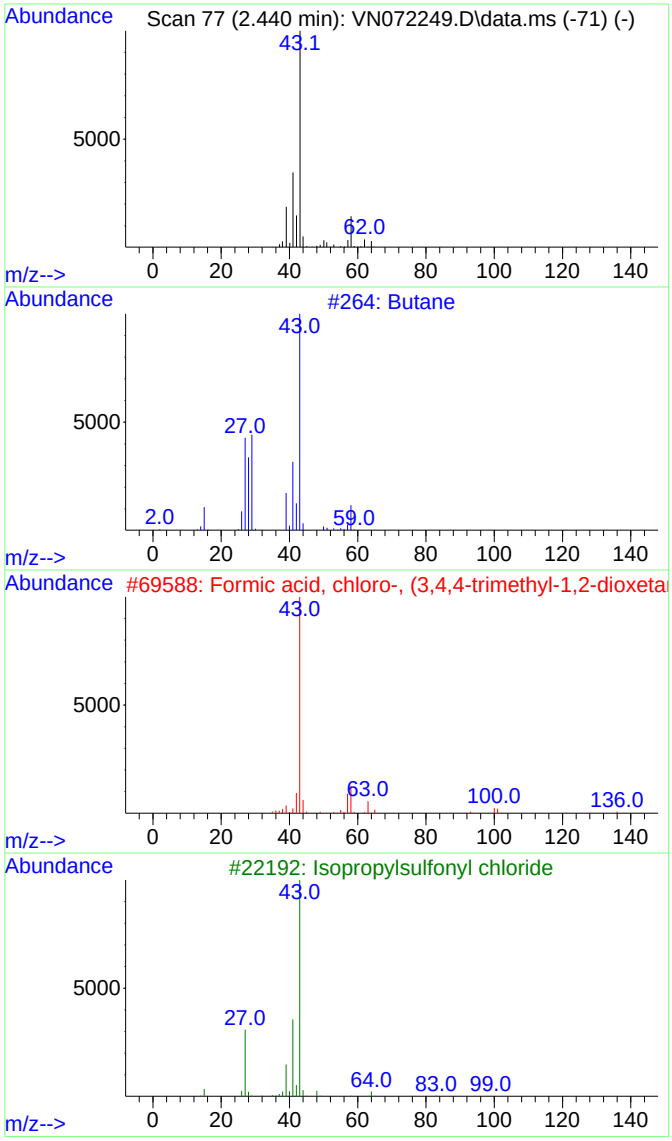
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

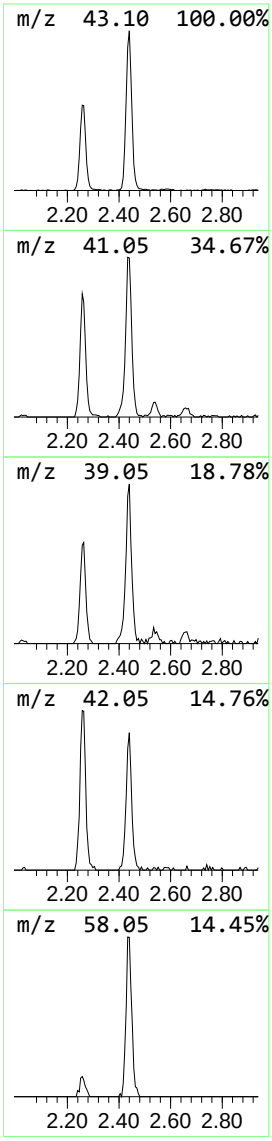
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.440	11.90 ug/l	214620	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane	58	C4H10	000106-97-8	64
2	Formic acid, chloro-, (3,4,4-tri...	194	C7H11ClO4	107323-92-2	36
3	Isopropylsulfonyl chloride	142	C3H7ClO2S	010147-37-2	23
4	Isobutane	58	C4H10	000075-28-5	9
5	1-Propanol, 2-chloro-	94	C3H7ClO	000078-89-7	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

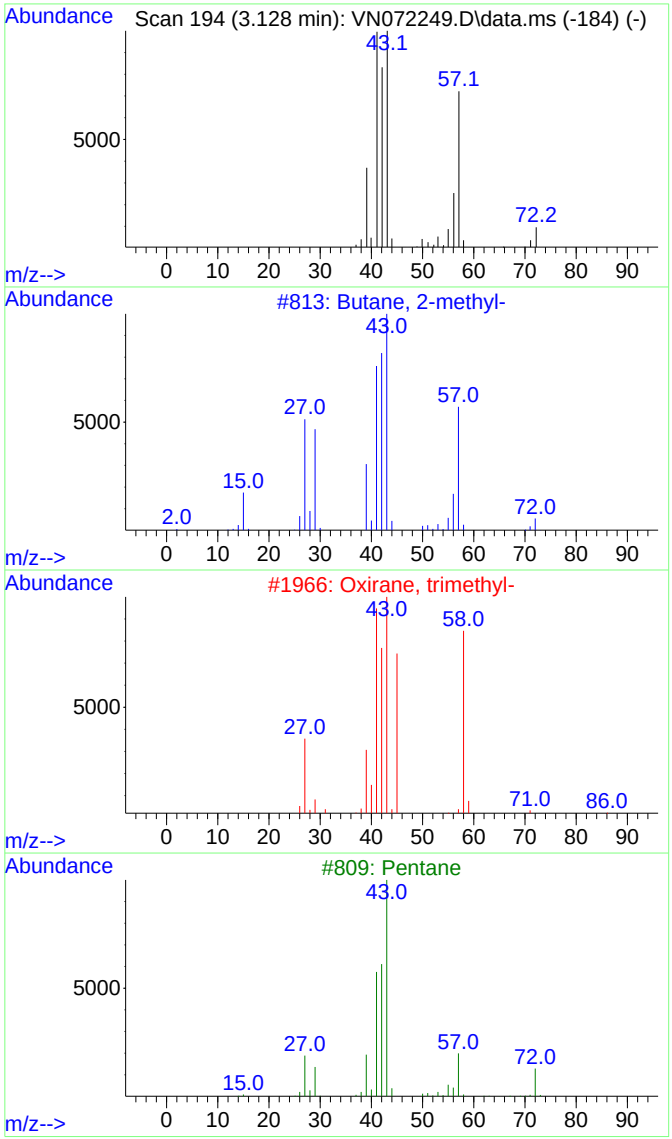
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

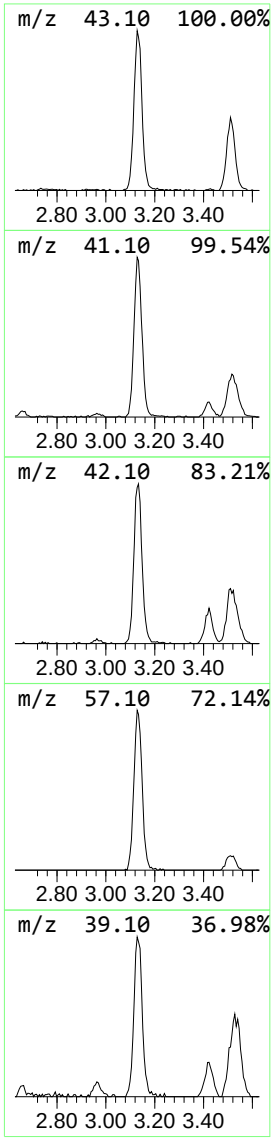
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	21.75 ug/l	392420	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	91
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
3	Pentane	72	C5H12	000109-66-0	33
4	3-Buten-1-ol	72	C4H8O	000627-27-0	28
5	1-Butene	56	C4H8	000106-98-9	10





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
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Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

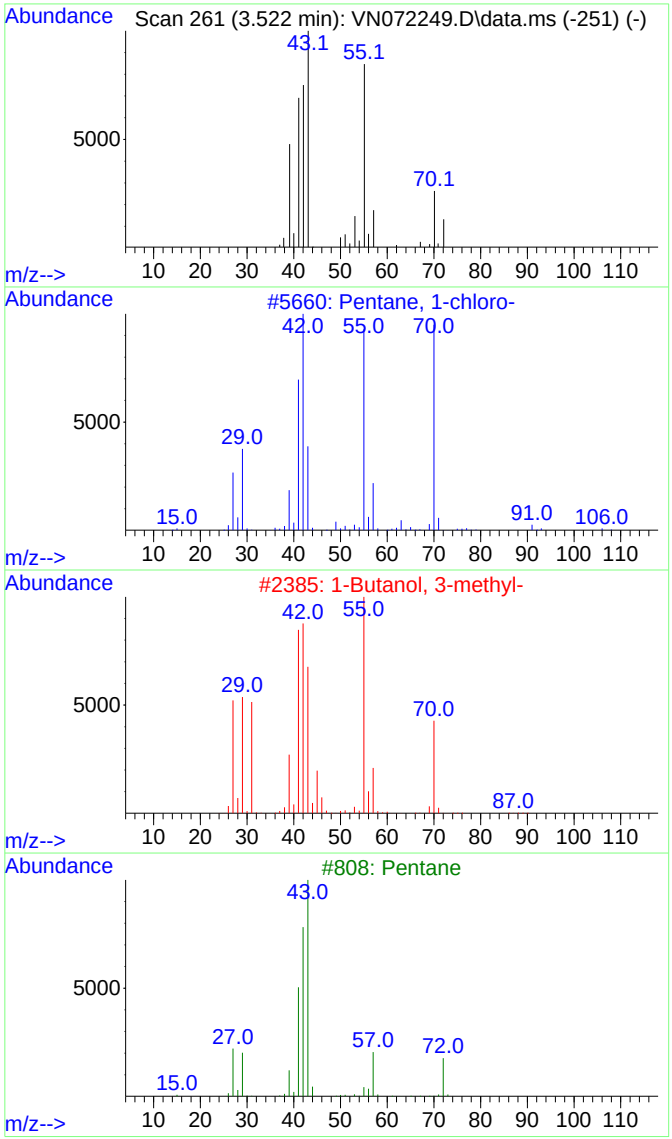
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

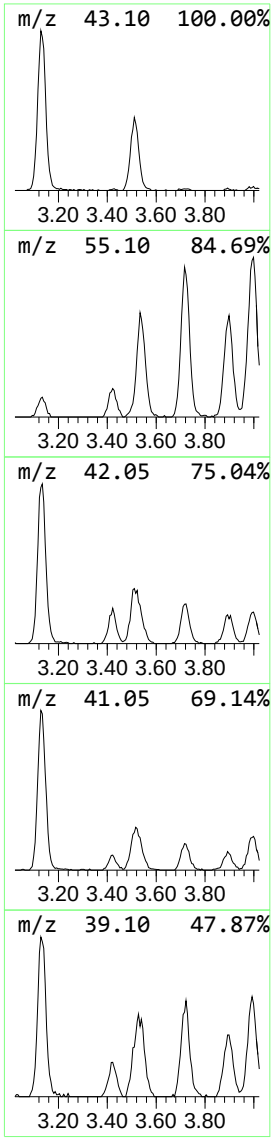
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Pentane, 1-chloro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.522	12.11 ug/l	218487	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 1-chloro-	106	C5H11Cl	000543-59-9	50
2	1-Butanol, 3-methyl-	88	C5H12O	000123-51-3	50
3	Pentane	72	C5H12	000109-66-0	47
4	2-Pentene, (Z)-	70	C5H10	000627-20-3	43
5	1-Pentene	70	C5H10	000109-67-1	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
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Sample : N2617-12
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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

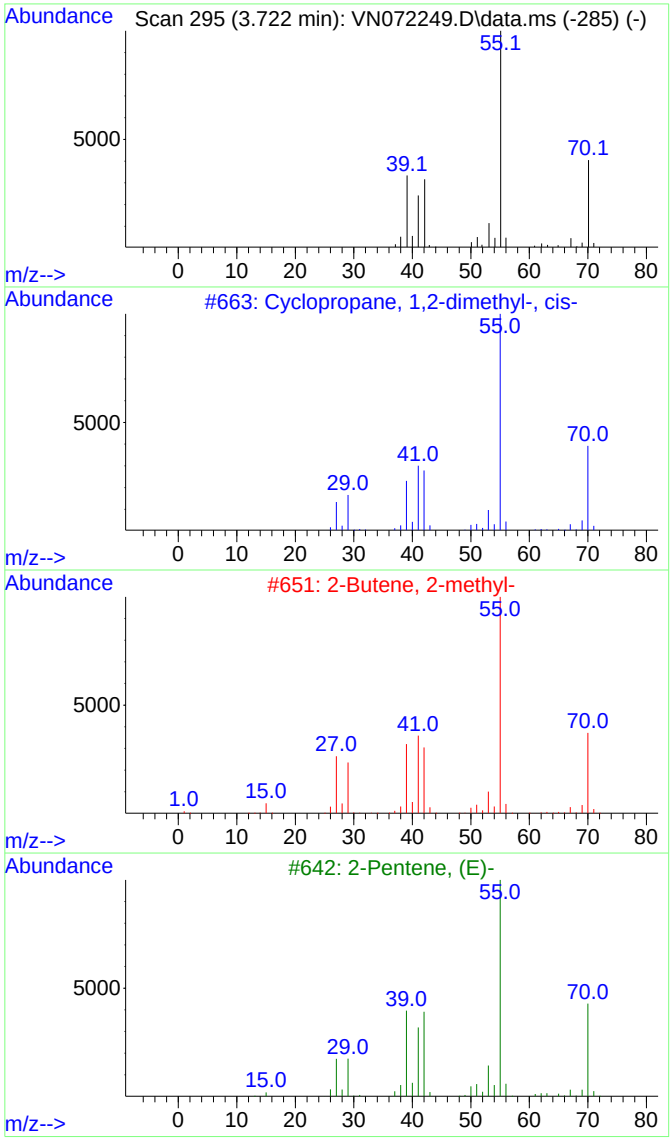
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

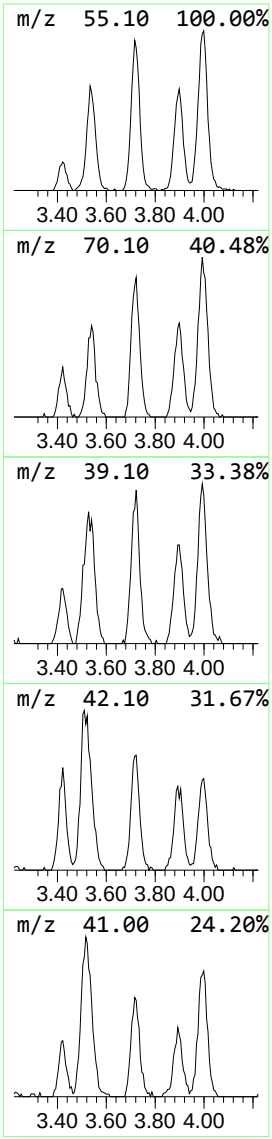
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopropane, 1,2-dimethyl-... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.722	9.34 ug/l	168487	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Butene, 2-methyl-	70	C5H10	000513-35-9	91
3	2-Pentene, (E)-	70	C5H10	000646-04-8	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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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

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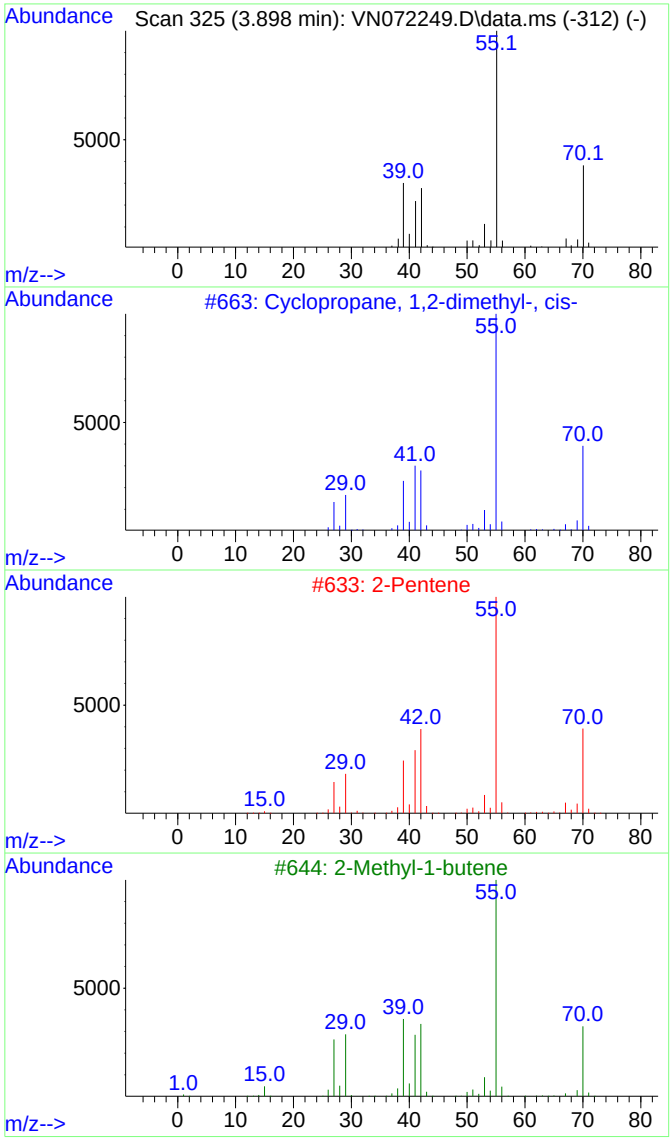
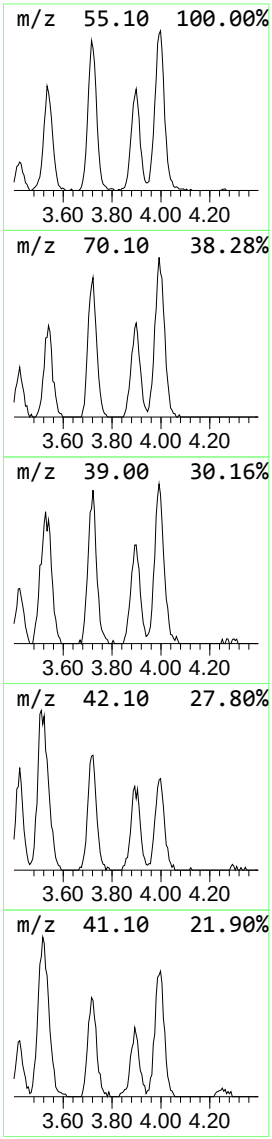
****

Peak Number 6 2-Pentene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.898	6.72 ug/l	121291	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	91
2	2-Pentene	70	C5H10	000109-68-2	91
3	2-Methyl-1-butene	70	C5H10	000563-46-2	91
4	1-Butene, 3-methyl-	70	C5H10	000563-45-1	86
5	2-Pentene, (E)-	70	C5H10	000646-04-8	86





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Instrument :
MSVOA_N
ClientSampleId :
MW-14D

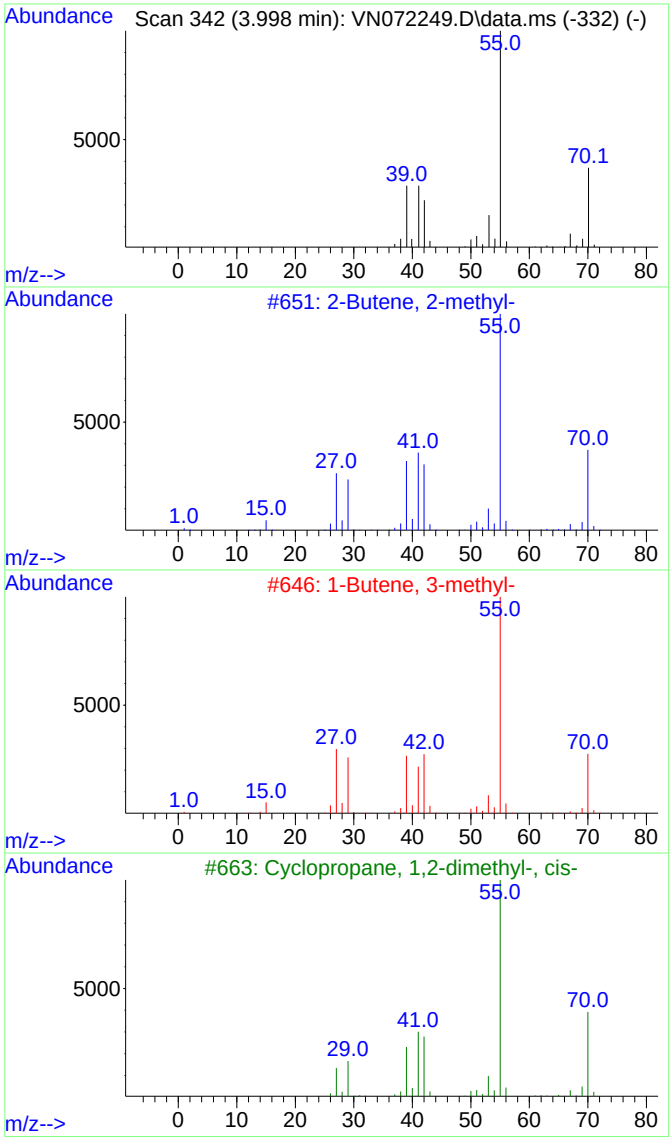
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

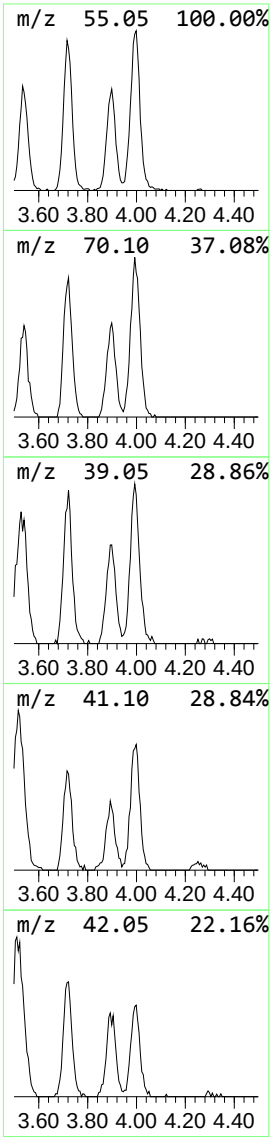
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2-Butene, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.998	11.01 ug/l	198572	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butene, 2-methyl-	70	C5H10	000513-35-9	87
2	1-Butene, 3-methyl-	70	C5H10	000563-45-1	80
3	Cyclopropane, 1,2-dimethyl-, cis-	70	C5H10	000930-18-7	72
4	2-Pentene, (E)-	70	C5H10	000646-04-8	72
5	2-Methyl-1-butene	70	C5H10	000563-46-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

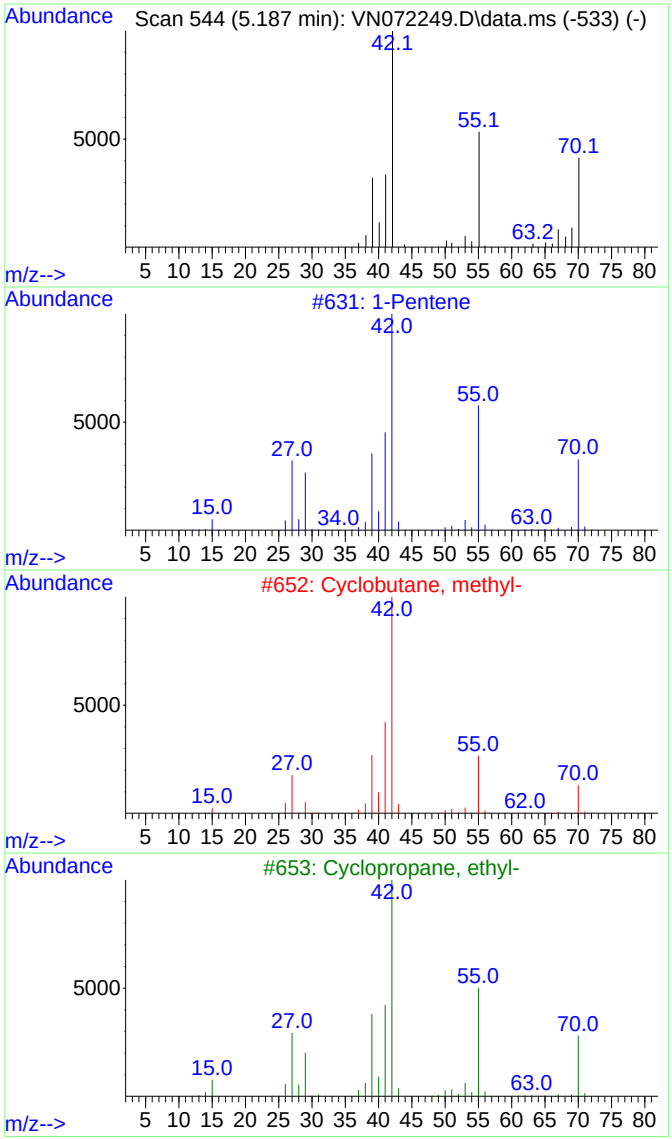
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

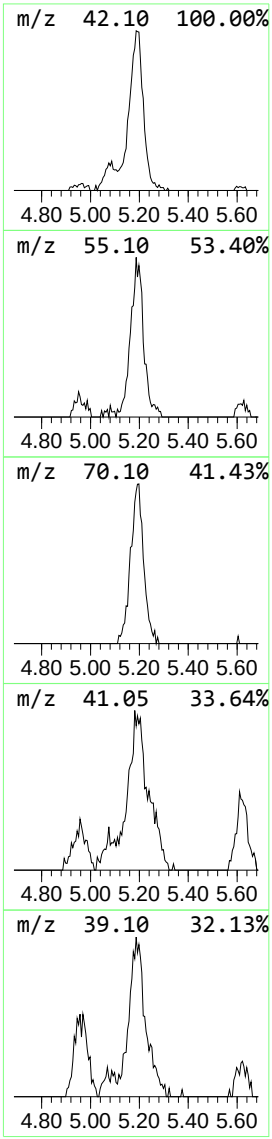
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Pentene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.187	10.15 ug/l	183078	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Pentene	70	C5H10	000109-67-1	78
2	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	45
4	2-Pentene	70	C5H10	000109-68-2	38
5	2-Pentene, (Z)-	70	C5H10	000627-20-3	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

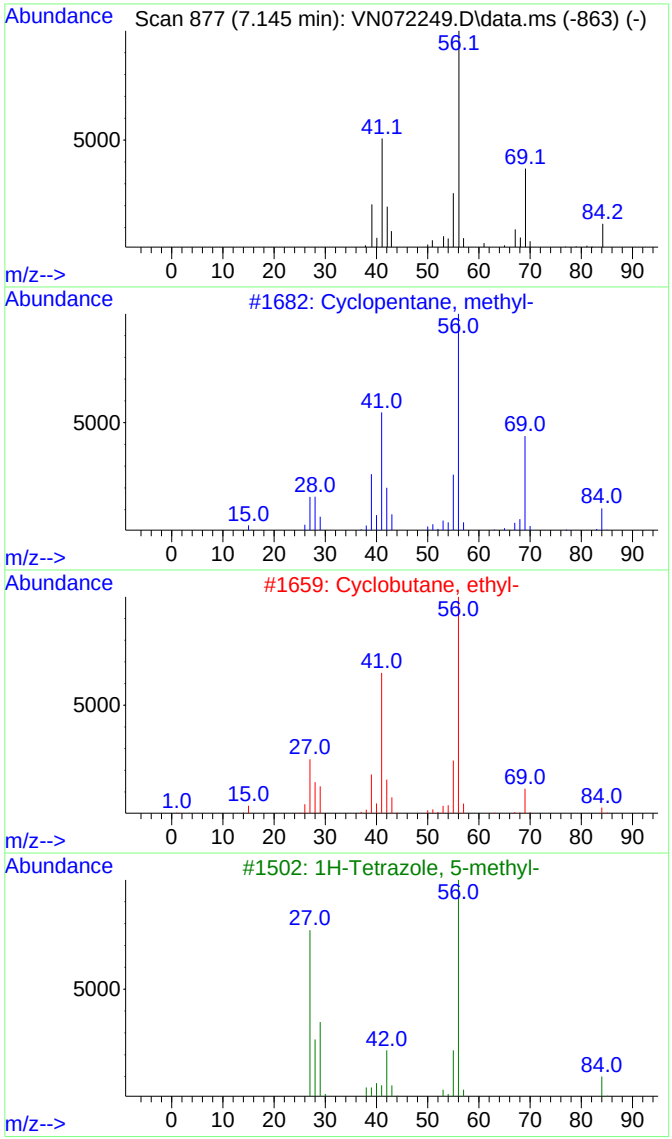
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.M
Quant Title : SW846 8260

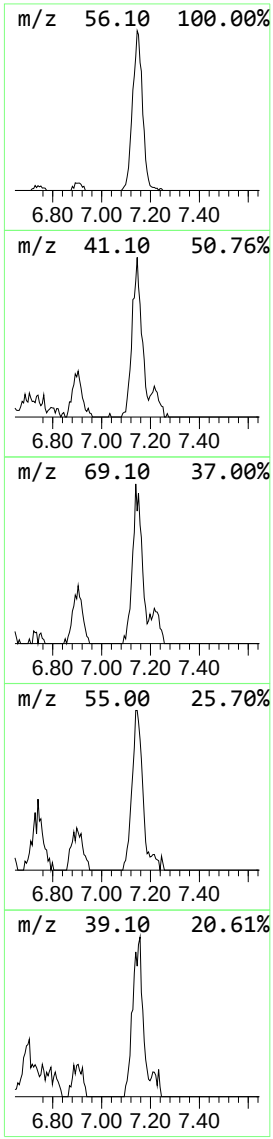
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Cyclopentane, methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	8.12 ug/l	146473	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	90
2	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
3	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64
4	2H-Pyran-2,6(3H)-dione, dihydro-...	142	C7H10O3	004160-82-1	59
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	43





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN042822\
Data File : VN072249.D
Acq On : 28 Apr 2022 19:47
Operator : JC\MD
Sample : N2617-12
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-14D

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N042622W.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
Sulfur dioxide	2.257	23.1	ug/l	416473	1	8.086	902088	50.0
Butane	2.440	11.9	ug/l	214620	1	8.086	902088	50.0
Butane, 2-methyl-	3.128	21.8	ug/l	392420	1	8.086	902088	50.0
Pentane, 1-chloro-	3.522	12.1	ug/l	218487	1	8.086	902088	50.0
Cyclopropane, 1...	3.722	9.3	ug/l	168487	1	8.086	902088	50.0
2-Pentene	3.898	6.7	ug/l	121291	1	8.086	902088	50.0
2-Butene, 2-met...	3.998	11.0	ug/l	198572	1	8.086	902088	50.0
1-Pentene	5.187	10.2	ug/l	183078	1	8.086	902088	50.0
Cyclopentane, m...	7.145	8.1	ug/l	146473	1	8.086	902088	50.0