LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

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\82N102022W.M
Title : SW846 8260

Signal : TIC: VN074982.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.242	191	202	218	rVB	2687308	6540659	3.73%	0.571%
2	5.288	537	550	555	rBV3	632416	2318896	1.32%	0.202%
3	5.353	556	561	590	rVB5	735082	3541998	2.02%	0.309%
4	5.824	623	641	659	rBV3	1813960	6394296	3.64%	0.558%
5	7.335	888	898	914	rBV	1964270	5772674	3.29%	0.504%
6	8.259	1045	1055	1062	rVV2	1216813	4445638	2.53%	0.388%
7	8.335	1062	1068	1078	rVB3	962775	2425659	1.38%	0.212%
8	8.612	1104	1115	1126	rBV	8028283	18870385	10.76%	1.648%
9	8.729	1126	1135	1139	rVV5	1285227	3662907	2.09%	0.320%
10	8.788	1140	1145	1152	rVV5	2041998	5154290	2.94%	0.450%
11	9.106	1189	1199	1212	rBV2	1076978	3069365	1.75%	0.268%
12	9.571	1265	1278	1280	rBV3	1046859	2213851	1.26%	0.193%
13	9.606	1280	1284	1301	rVB	1439006	3347245	1.91%	0.292%
14	10.106	1362	1369	1373	rBV	1369892	2682007	1.53%	0.234%
15	10.570	1441	1448	1454	rBV2	2158324	4066243	2.32%	0.355%
16	10.635	1454	1459	1468	rVV2	699409	1928137	1.10%	0.168%
17	10.988	1512	1519	1528	rVB3	968144	2460674	1.40%	0.215%
18	11.865	1660	1668	1674	rBV4	1146019	2385509	1.36%	0.208%
19	11.965	1674	1685	1695	rBV2	56233982	101680604	57.96%	8.878%
20	12.076	1695	1704	1714	rBV3	87857349	175431999	100.00%	15.318%
21	12.400	1748	1759	1766	rBV	4162080	7297337	4.16%	0.637%
22	12.700	1804	1810	1817	rVB	4874239	7979471	4.55%	0.697%
23	12.853	1826	1836	1847	rBV2	1361286	2760703	1.57%	0.241%
24	13.041	1857	1868	1873	rBV	8481674	13969950	7.96%	1.220%
25	13.100	1873	1878	1881	rVV	15220480	25845218	14.73%	2.257%
26	13.135	1881	1884	1887	rVV	18506445	27633014	15.75%	2.413%
27	13.176	1887	1891	1899	rVB	26469935	40481849	23.08%	3.535%
28	13.341	1911	1919	1928	rBV	25596843	43431177	24.76%	3.792%
29	13.488	1928	1944	1951	rBV3	93782668	161635955	92.14%	14.114%
30	13.611	1957	1965	1971	rVB3	786930	2005545	1.14%	0.175%
31	13.823	1990	2001	2011	rBV	35928957	62643730	35.71%	5.470%
32	13.953	2017	2023	2025	rBV	6288205	9326420	5.32%	0.814%
33	14.000	2025	2031	2046	rVB3	54198048	108350309	61.76%	9.461%
34	14.117	2046	2051	2056	rBV	1222810	1969905	1.12%	0.172%
35	14.182	2056	2062	2068	rVV2	5789711	10180573	5.80%	0.889%
36	14.247	2068	2073	2076	rVV	5967597	10399868	5.93%	0.908%

LSC Area Percent Report

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Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

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\82N102022W.M
Title : SW846 8260

37	14.276	2076	2078	2082	rVV	4758599	5967244	3.40%	0.521%
38	14.335	2082	2088	2094	rVV	14065978	22111449	12.60%	1.931%
39	14.400	2094	2099	2102	rVV	3590441	5874609	3.35%	0.513%
40	14.447	2102	2107	2116	rVB	14656042	24626434	14.04%	2.150%
41	14.576	2124	2129	2135	rVB2	2550803	4068909	2.32%	0.355%
42	14.658	2135	2143	2146	rBV	9168055	15762652	8.99%	1.376%
43	14.694	2146	2149	2154	rVV	9438831	14451946	8.24%	1.262%
44	14.929	2183	2189	2195	rBV	10302920	16546718	9.43%	1.445%
45	15.053	2201	2210	2216	rBV2	17609459	37671424	21.47%	3.289%
46	15.117	2216	2221	2228	rVB3	2257200	4445328	2.53%	0.388%
47	15.211	2230	2237	2244	rBV2	3792384	7109949	4.05%	0.621%
48	15.323	2244	2256	2260	rBV4	3167129	8084991	4.61%	0.706%
49	15.441	2268	2276	2284	rVB3	2569168	6517195	3.71%	0.569%
50	15.641	2302	2310	2321	rVB2	32451198	65540439	37.36%	5.723%
51	15.747	2321	2328	2334	rVV	2520289	5099624	2.91%	0.445%
52	15.811	2334	2339	2353	rVB	742709	1797994	1.02%	0.157%
53	15.947	2354	2362	2370	rBV	1314387	2595602	1.48%	0.227%
54	16.129	2383	2393	2410	rBV2	729236	2675863	1.53%	0.234%

Sum of corrected areas: 1145252430

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Operator : JC\MD
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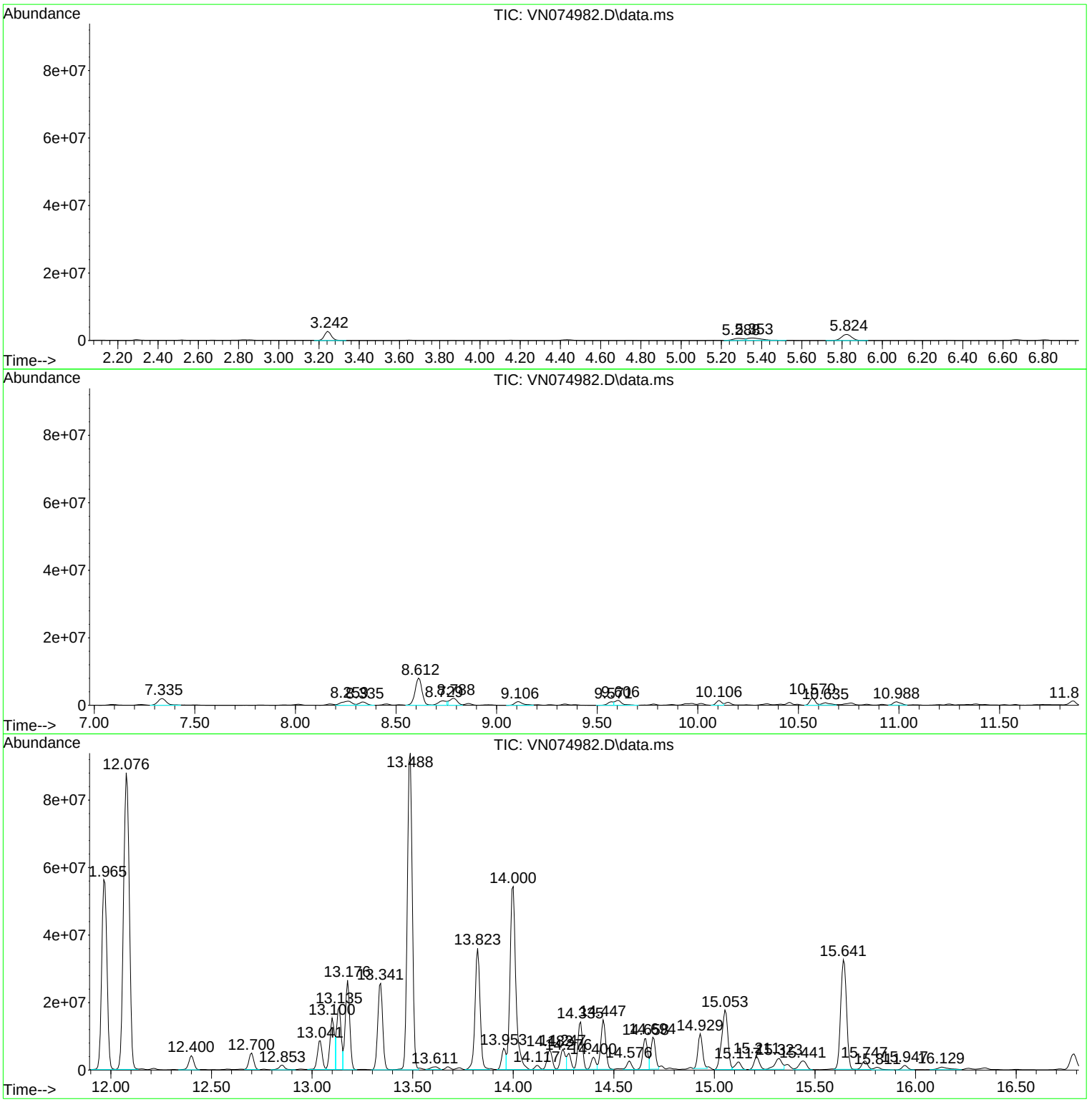
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
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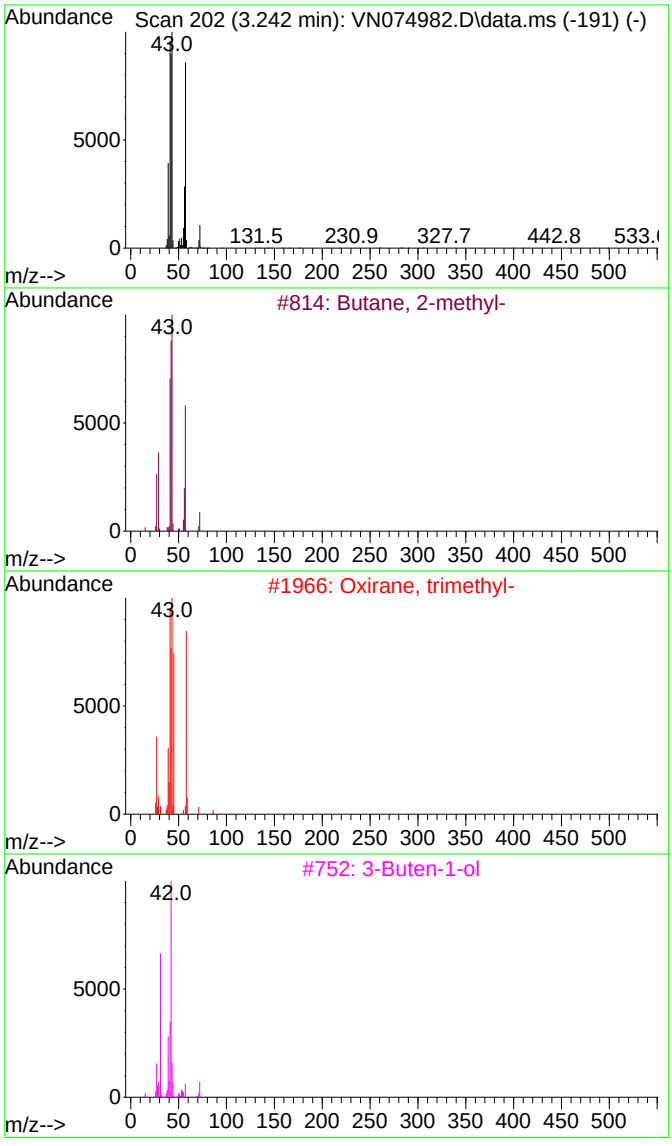
Quant Title : SW846 8260

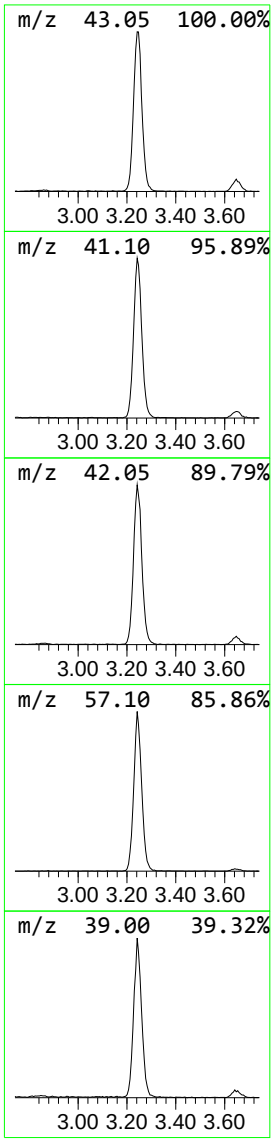
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.242	73.56 ug/l	6540660	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	64
2	Oxirane, trimethyl-	86	C5H10O	005076-19-7	25
3	3-Buten-1-ol	72	C4H8O	000627-27-0	23
4	1-Propene, 2-methyl-	56	C4H8	000115-11-7	22
5	Pentane	72	C5H12	000109-66-0	16





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Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

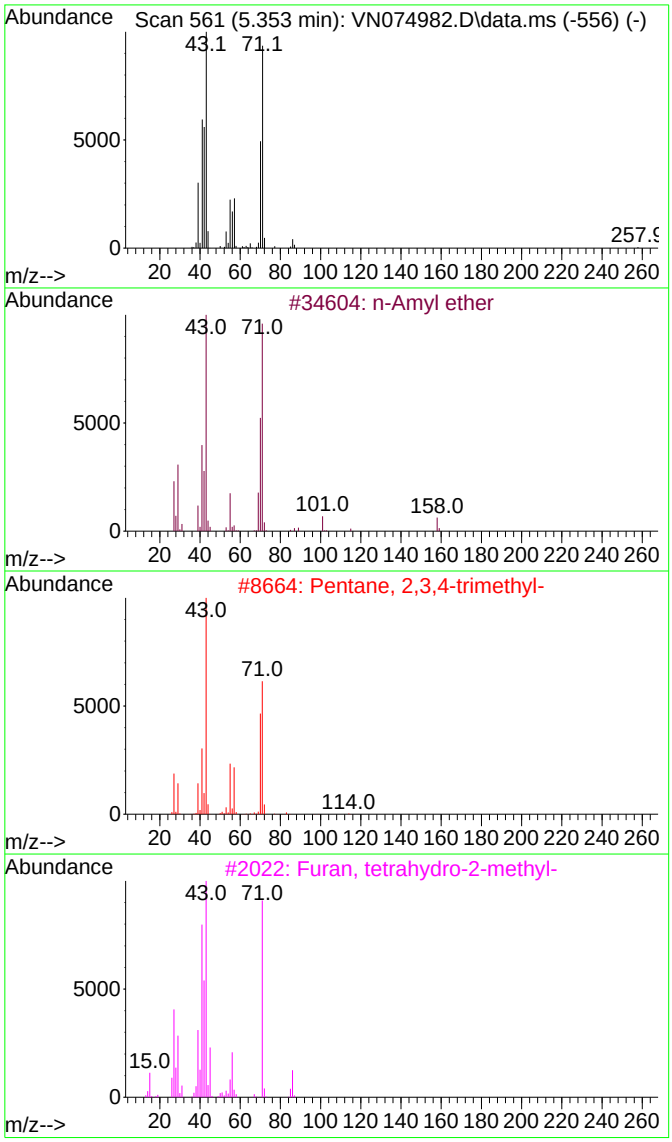
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

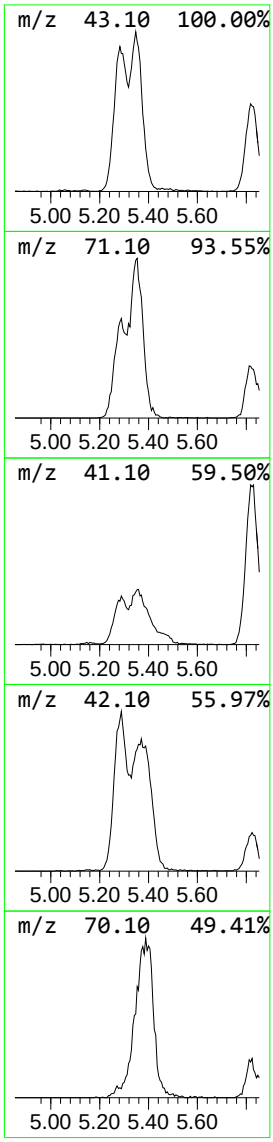
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 n-Amyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.353	39.84 ug/l	3542000	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Amyl ether	158	C10H22O	000693-65-2	64
2	Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	59
3	Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	47
4	Carbonic acid, 2-methylbutyl neo...	202	C11H22O3	1010331-42-9	40
5	Decane, 4-methyl-	156	C11H24	002847-72-5	38





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

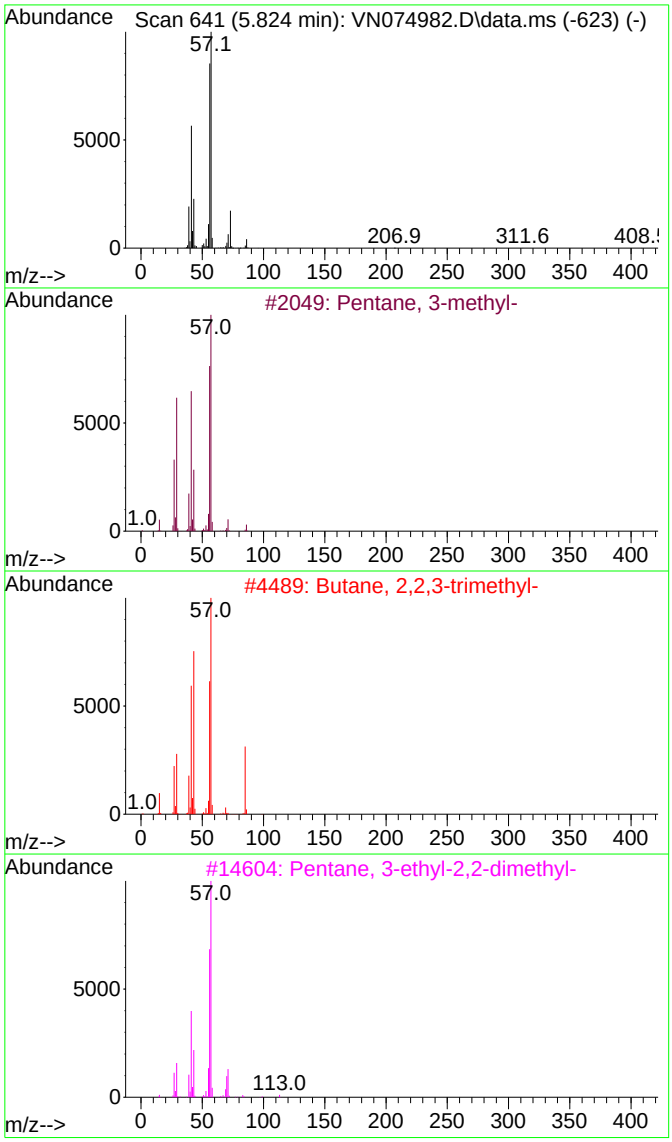
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

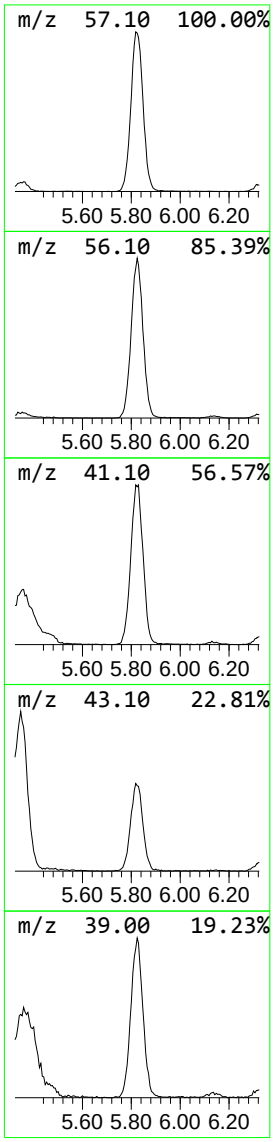
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.824	71.92 ug/l	6394300	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	87
2	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	72
3	Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	56
4	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	50
5	3,4-Dimethyldihydrofuran-2,5-dione	128	C6H8O3	007475-92-5	40





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

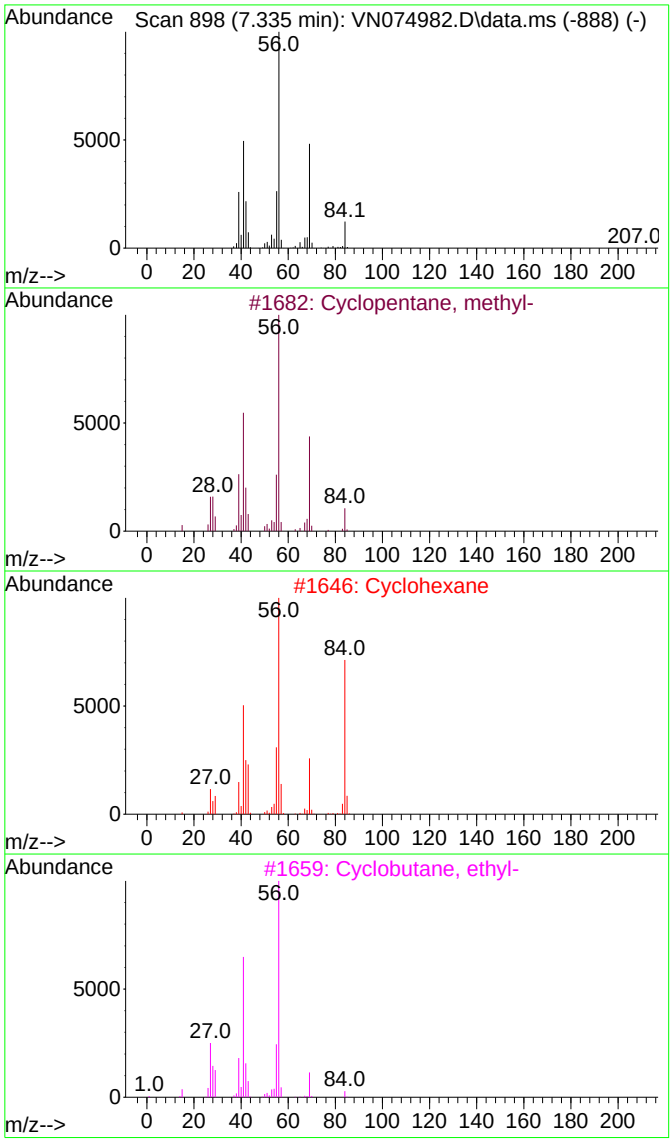
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

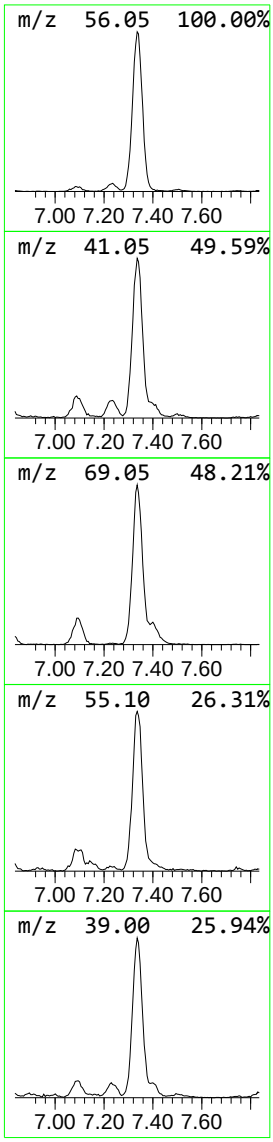
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.335	64.93 ug/l	5772670	Pentafluorobenzene	8.229

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2	Cyclohexane	84	C6H12	000110-82-7	78
3	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
4	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	72
5	1-Pentene, 2-methyl-	84	C6H12	000763-29-1	64





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Operator : JC\MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

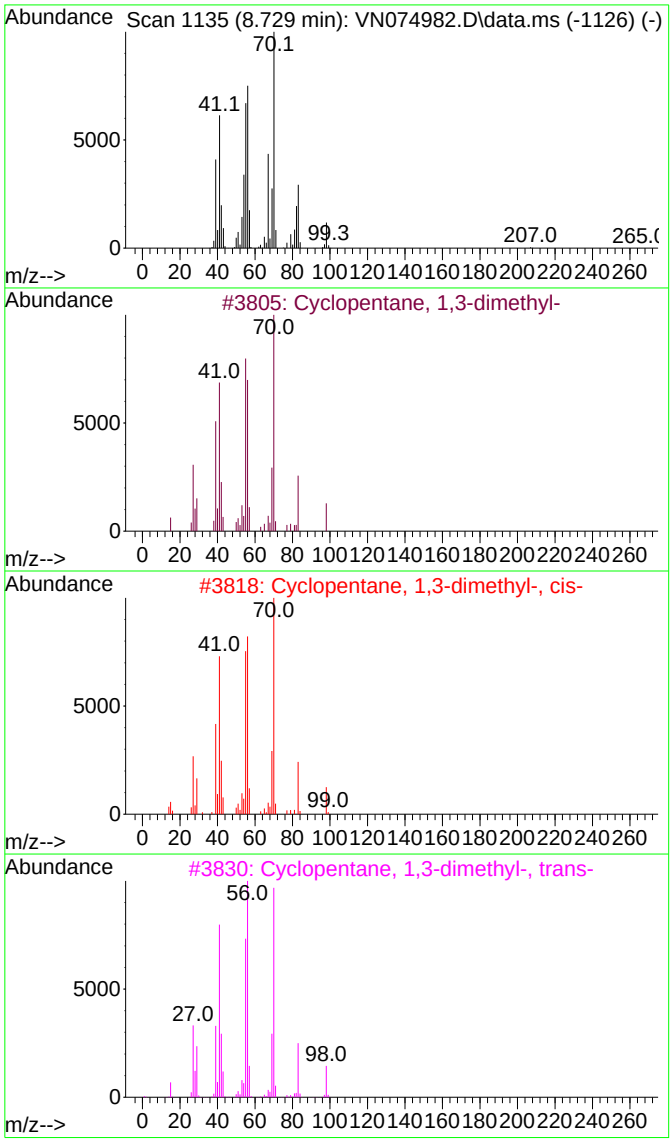
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

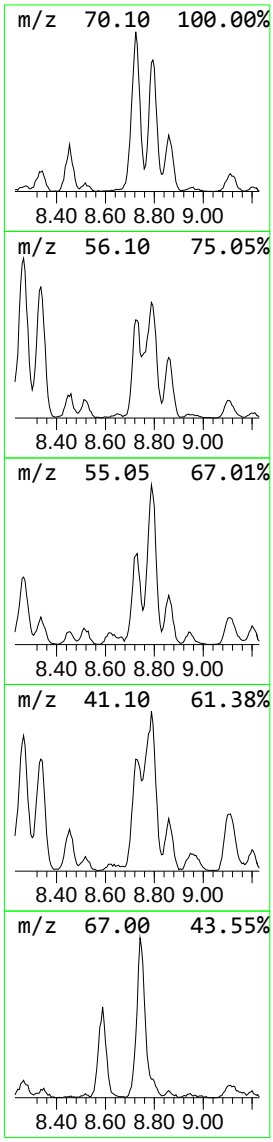
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Cyclopentane, 1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.729	59.67 ug/l	3662910	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,3-dimethyl-	98	C7H14	002453-00-1	93
2	Cyclopentane, 1,3-dimethyl-, cis-	98	C7H14	002532-58-3	76
3	Cyclopentane, 1,3-dimethyl-, trans-	98	C7H14	001759-58-6	64
4	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	60
5	E-11,13-Tetradecadien-1-ol	210	C14H26O	1000131-00-3	47





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Acq On : 24 Oct 2022 14:36
Operator : JC\MD
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

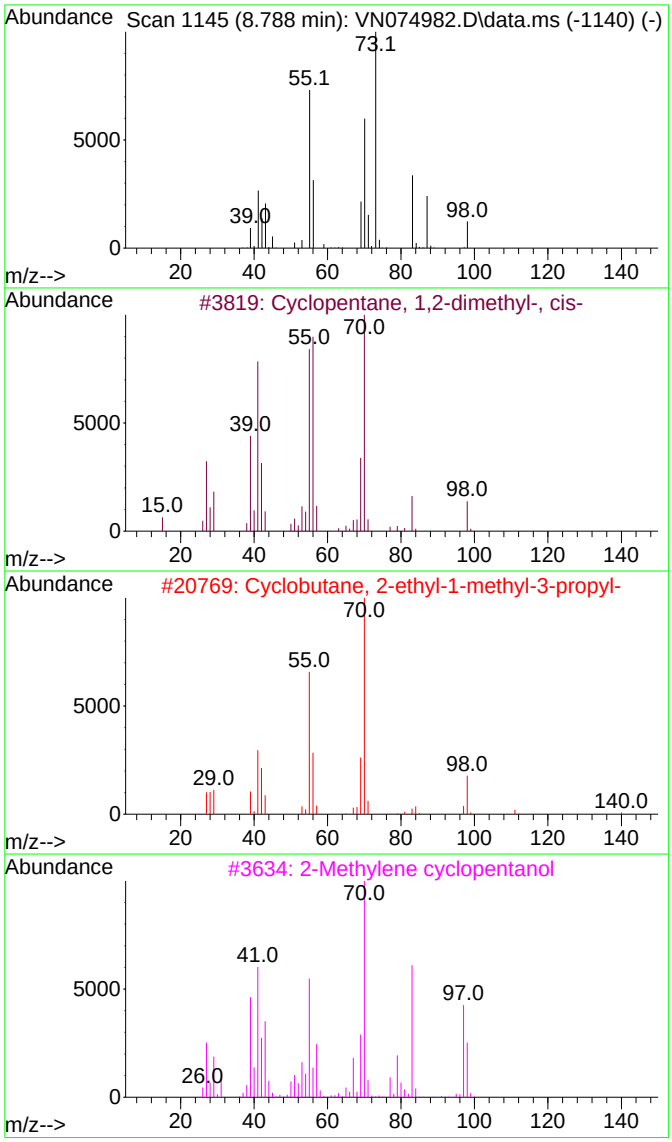
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

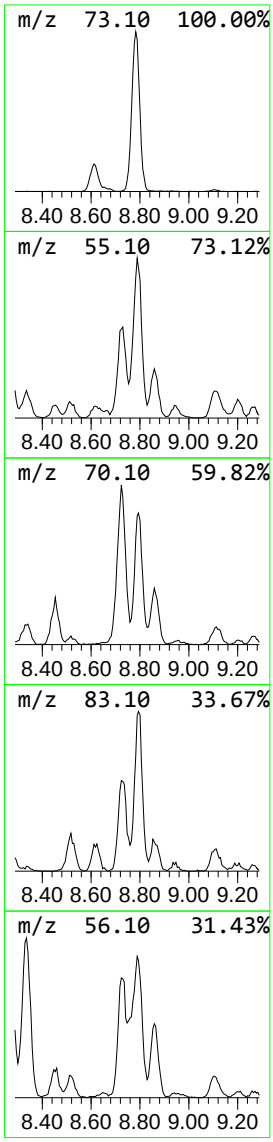
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 unknown8.788 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.788	83.96 ug/l	5154290	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 1,2-dimethyl-, cis-	98	C7H14	001192-18-3	43
2	Cyclobutane, 2-ethyl-1-methyl-3-...	140	C10H20	061233-72-5	32
3	2-Methylene cyclopentanol	98	C6H10O	020461-31-8	32
4	Chloroacetic acid, heptyl ester	192	C9H17ClO2	034589-22-5	32
5	1-Heptene, 5-methyl-	112	C8H16	013151-04-7	25





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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

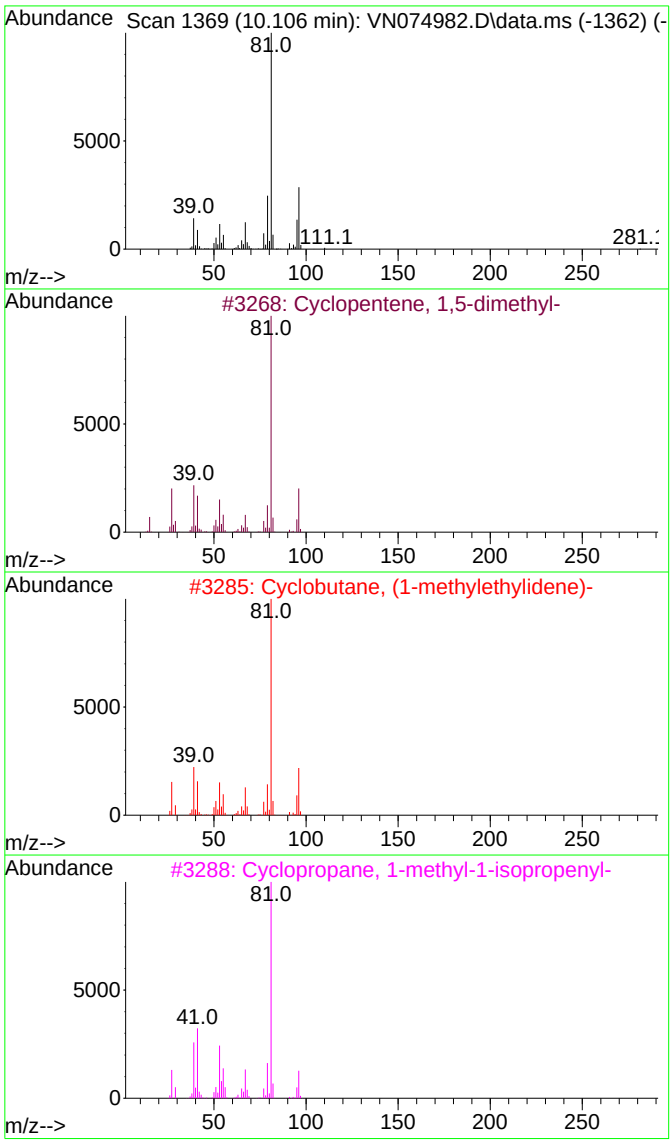
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

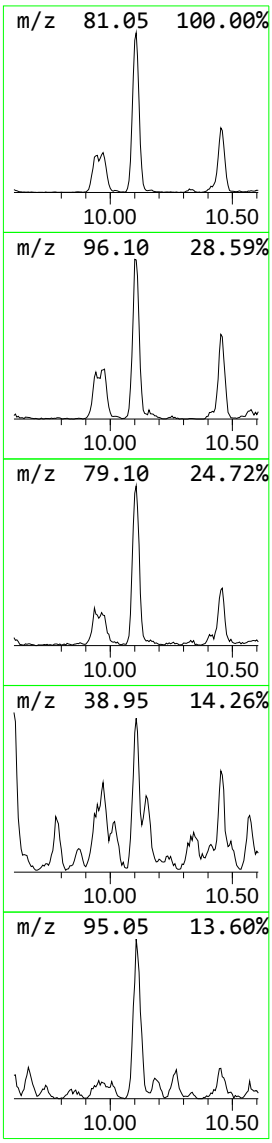
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Cyclopentene, 1,5-dimethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.106	43.69 ug/l	2682010	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentene, 1,5-dimethyl-	96	C7H12	016491-15-9	87
2	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	87
3	Cyclopropane, 1-methyl-1-isoprop...	96	C7H12	003422-07-9	86
4	3,5-Dimethylcyclopentene	96	C7H12	007459-71-4	78
5	1,4-Pentadiene, 3,3-dimethyl-	96	C7H12	001112-35-2	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
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ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
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MW-2

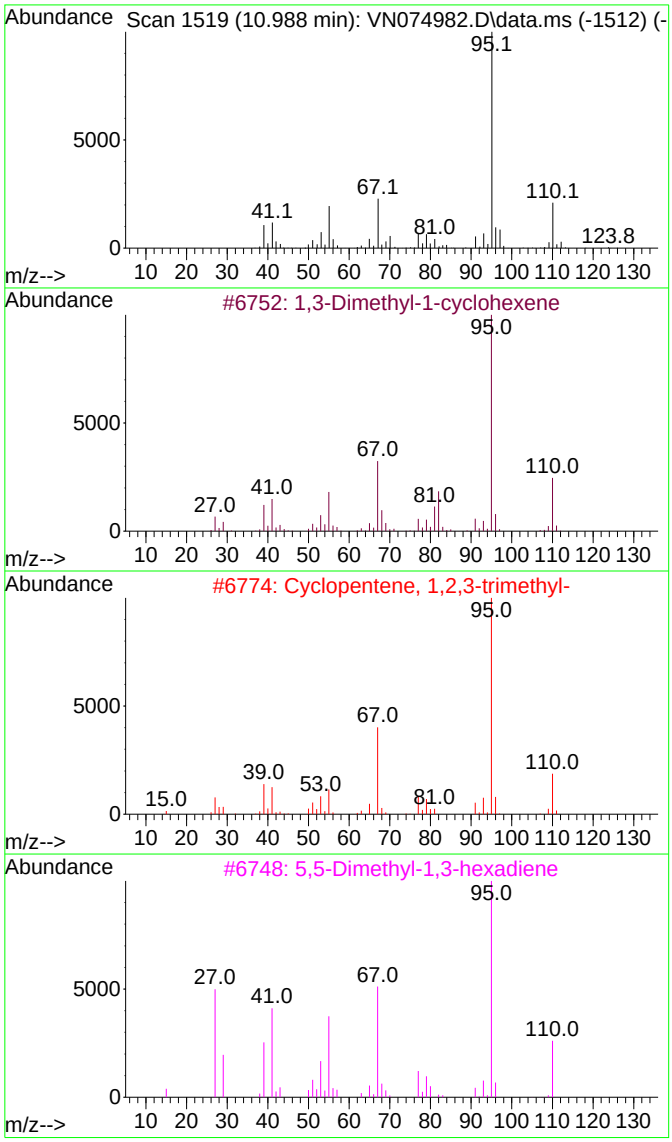
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

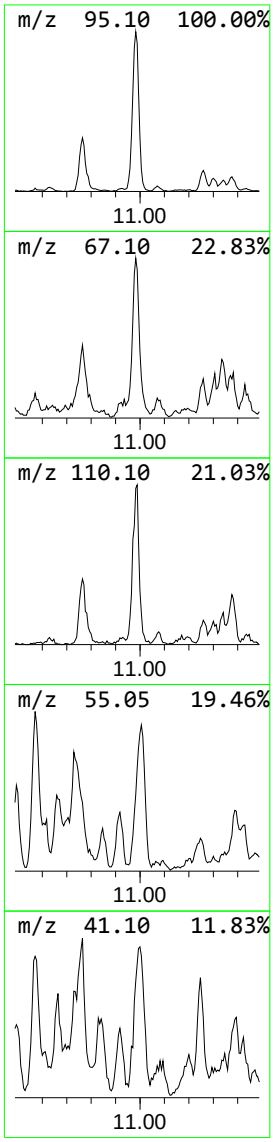
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1,3-Dimethyl-1-cyclohexene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	51.58 ug/l	2460670	Chlorobenzene-d5	11.870

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	87
2	Cyclopentene, 1,2,3-trimethyl-	110	C8H14	000473-91-6	87
3	5,5-Dimethyl-1,3-hexadiene	110	C8H14	001515-79-3	83
4	1,4-Pentadiene, 2,3,3-trimethyl-	110	C8H14	000756-02-5	78
5	Cyclohexene, 3,5-dimethyl-	110	C8H14	000823-17-6	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

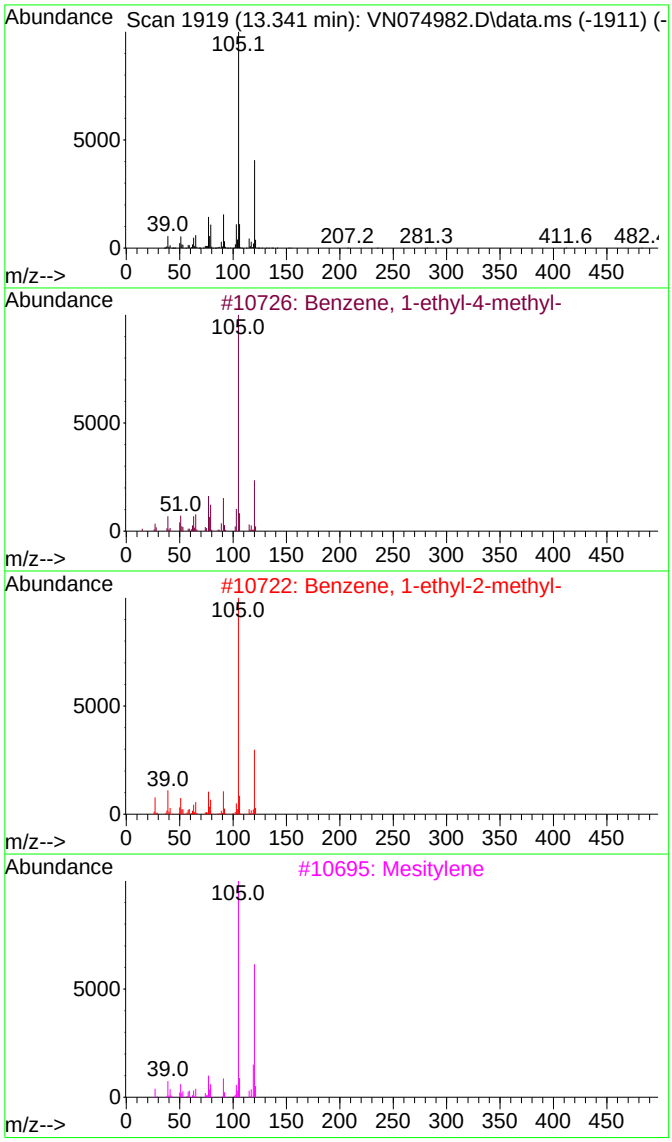
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

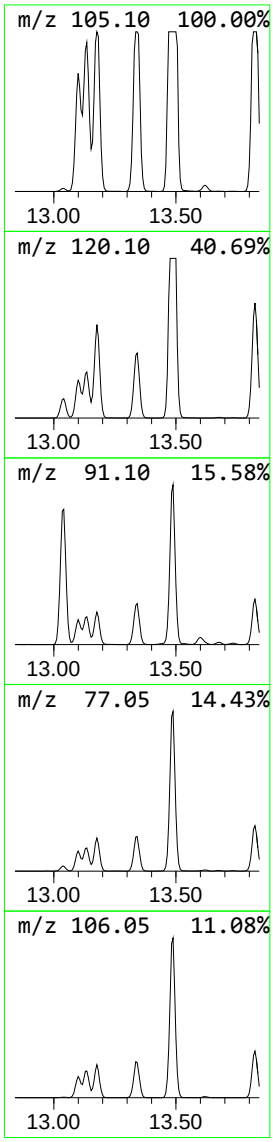
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Benzene, 1-ethyl-4-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.341	34.67 ug/l	43431200	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
2	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
3	Mesitylene	120	C9H12	000108-67-8	91
4	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

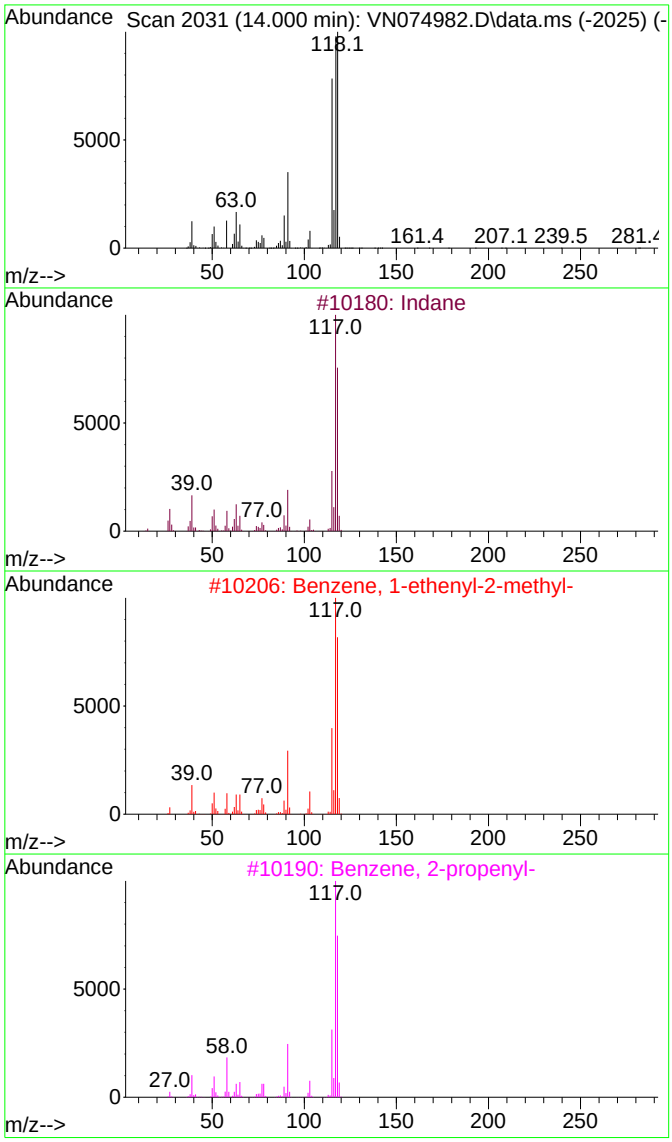
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

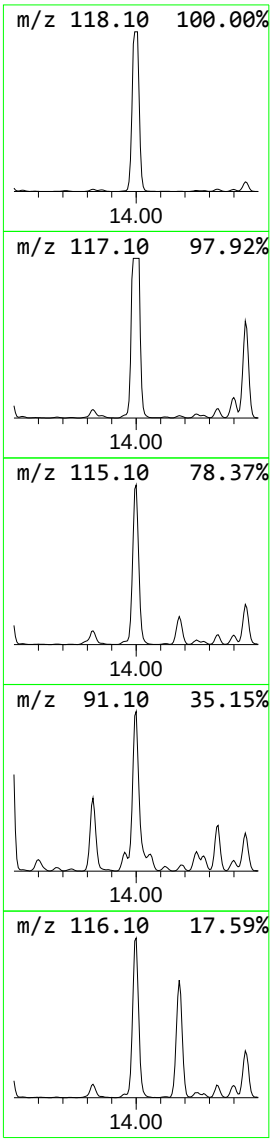
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Indane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.000	86.48 ug/l	108350000	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indane	118	C9H10	000496-11-7	83
2	Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	64
3	Benzene, 2-propenyl-	118	C9H10	000300-57-2	64
4	Benzene, 1-propenyl-	118	C9H10	000637-50-3	53
5	Benzene, 1-ethenyl-4-methyl-	118	C9H10	000622-97-9	52





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102422\
Data File : VN074982.D
Acq On : 24 Oct 2022 14:36
Operator : JC\MD
Sample : N5222-04
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.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-	3.242	73.6	ug/l	6540660	1	8.229	4445640	50.0
n-Amyl ether	5.353	39.8	ug/l	3542000	1	8.229	4445640	50.0
Pentane, 3-methyl-	5.824	71.9	ug/l	6394300	1	8.229	4445640	50.0
Cyclopentane, m...	7.335	64.9	ug/l	5772670	1	8.229	4445640	50.0
Cyclopentane, 1...	8.729	59.7	ug/l	3662910	2	9.106	3069370	50.0
unknown8.788	8.788	84.0	ug/l	5154290	2	9.106	3069370	50.0
Cyclopentene, 1...	10.106	43.7	ug/l	2682010	2	9.106	3069370	50.0
1,3-Dimethyl-1-...	10.988	51.6	ug/l	2460670	3	11.870	2385510	50.0
Benzene, 1-ethy...	13.341	34.7	ug/l	43431200	4	13.794	62643700	50.0
Indane	14.000	86.5	ug/l	108350000	4	13.794	62643700	50.0