LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-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 : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Title : SW846 8260

Signal : TIC: VN072460.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.263	37	47	55	rBV4	58072	251095	1.55%	0.223%
2	3.128	185	194	206	rVB	320844	730857	4.52%	0.649%
3	3.510	250	259	276	rVB	95620	246351	1.53%	0.219%
4	5.181	530	543	556	rVB4	92033	477915	2.96%	0.424%
5	5.622	605	618	631	rBV2	83481	279803	1.73%	0.248%
6	7.145	866	877	888	rBV2	174956	533053	3.30%	0.473%
7	8.016	1015	1025	1030	rBV	145366	348258	2.16%	0.309%
8	8.087	1030	1037	1046	rVV2	366488	936220	5.80%	0.831%
9	8.439	1088	1097	1108	rBV3	232372	707217	4.38%	0.628%
10	8.581	1108	1121	1128	rBV6	93783	299146	1.85%	0.266%
11	8.963	1178	1186	1199	rBV	392315	868046	5.37%	0.771%
12	9.457	1256	1270	1277	rBV3	84259	256447	1.59%	0.228%
13	9.969	1350	1357	1362	rBV	120110	236104	1.46%	0.210%
14	10.439	1429	1437	1441	rBV	585457	1083105	6.71%	0.962%
15	10.504	1441	1448	1462	rVB	5318593	9774622	60.51%	8.681%
16	11.739	1650	1658	1667	rBV	534697	956270	5.92%	0.849%
17	11.839	1667	1675	1686	rVV	9544657	16152826	100.00%	14.345%
18	11.951	1686	1694	1705	rVB	7295521	14340311	88.78%	12.736%
19	12.275	1737	1749	1767	rBV	7160421	12205381	75.56%	10.840%
20	12.575	1788	1800	1807	rVB	662377	1094401	6.78%	0.972%
21	12.727	1818	1826	1835	rVB	455018	754123	4.67%	0.670%
22	12.916	1851	1858	1863	rBV	1607633	2580697	15.98%	2.292%
23	12.980	1863	1869	1872	rVV	2723308	4625311	28.63%	4.108%
24	13.010	1872	1874	1878	rVV	1492755	2158222	13.36%	1.917%
25	13.057	1878	1882	1892	rVB	2547872	3958127	24.50%	3.515%
26	13.216	1902	1909	1920	rBV	2320227	3815105	23.62%	3.388%
27	13.363	1926	1934	1941	rBV	6669808	10827350	67.03%	9.616%
28	13.492	1948	1956	1962	rVB3	85275	204218	1.26%	0.181%
29	13.698	1980	1991	2001	rBV2	1673743	3575611	22.14%	3.176%
30	13.833	2007	2014	2016	rBV	457201	710203	4.40%	0.631%
31	13.869	2016	2020	2037	rVV2	2554139	5712001	35.36%	5.073%
32	14.057	2046	2052	2058	rVV2	265384	513913	3.18%	0.456%
33	14.127	2058	2064	2067	rVV	435252	752669	4.66%	0.668%
34	14.157	2067	2069	2073	rVV	255242	305307	1.89%	0.271%
35	14.210	2073	2078	2084	rVV	994376	1539499	9.53%	1.367%
36	14.274	2084	2089	2092	rVV	149330	237277	1.47%	0.211%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-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 : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N051022W.M
Title : SW846 8260

37	14.321	2092	2097	2106	rVB2	579117	964587	5.97%	0.857%
38	14.457	2114	2120	2125	rVB2	110407	174121	1.08%	0.155%
39	14.533	2125	2133	2136	rBV	465269	732703	4.54%	0.651%
40	14.574	2136	2140	2145	rVB	636630	946974	5.86%	0.841%
41	14.804	2174	2179	2185	rBV	421025	655498	4.06%	0.582%
42	14.927	2191	2200	2206	rBV2	820214	1692348	10.48%	1.503%
43	15.080	2217	2226	2234	rBV2	177390	322175	1.99%	0.286%
44	15.192	2234	2245	2249	rBV5	85509	225745	1.40%	0.200%
45	15.304	2256	2264	2273	rVB3	84214	200505	1.24%	0.178%
46	15.498	2289	2297	2305	rBV	1224350	2322258	14.38%	2.062%
47	16.610	2479	2486	2499	rVB	139655	315163	1.95%	0.280%

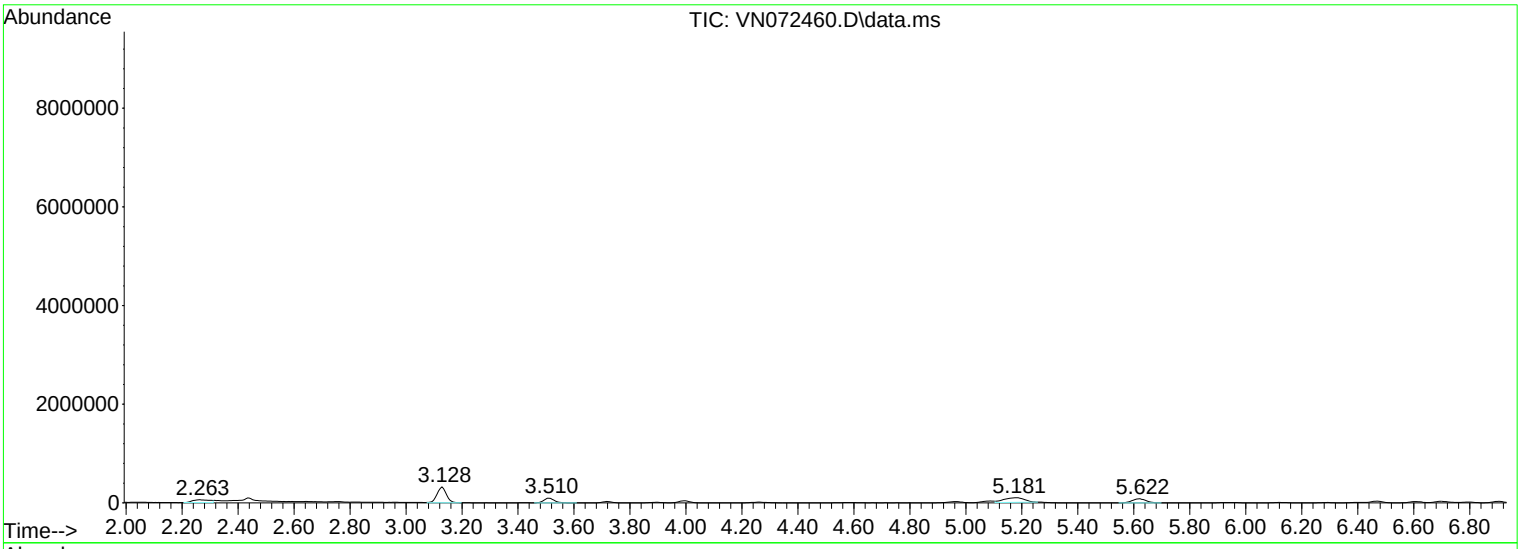
Sum of corrected areas: 112599138

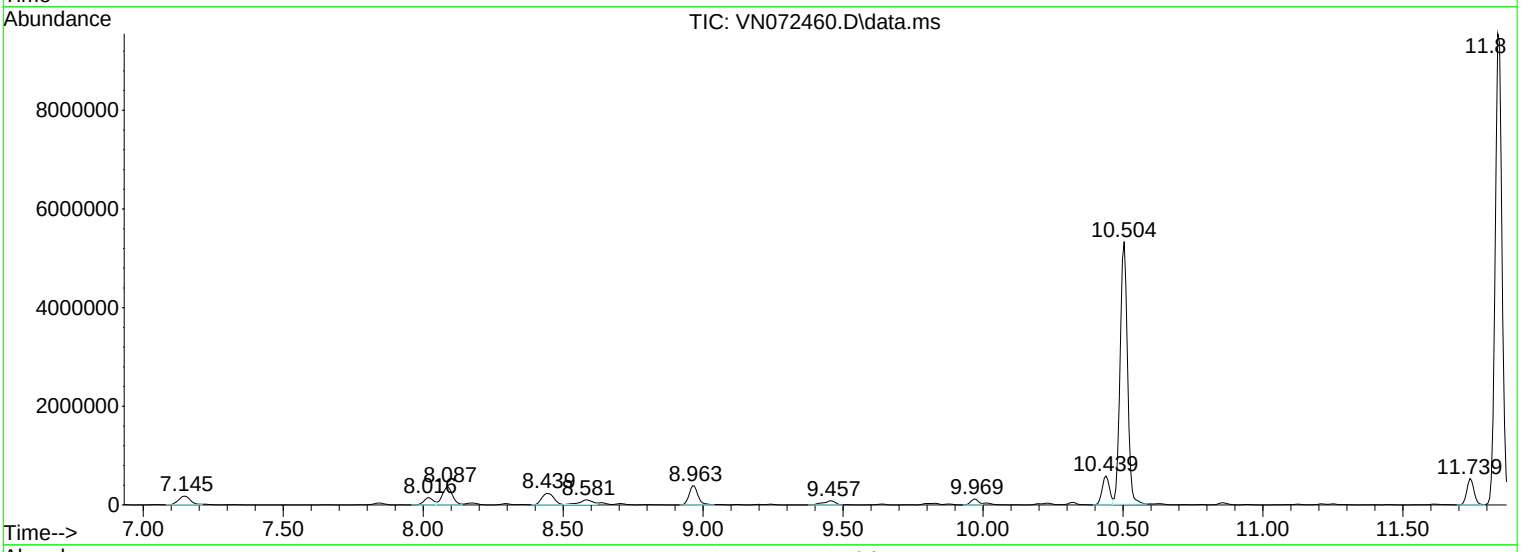
Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

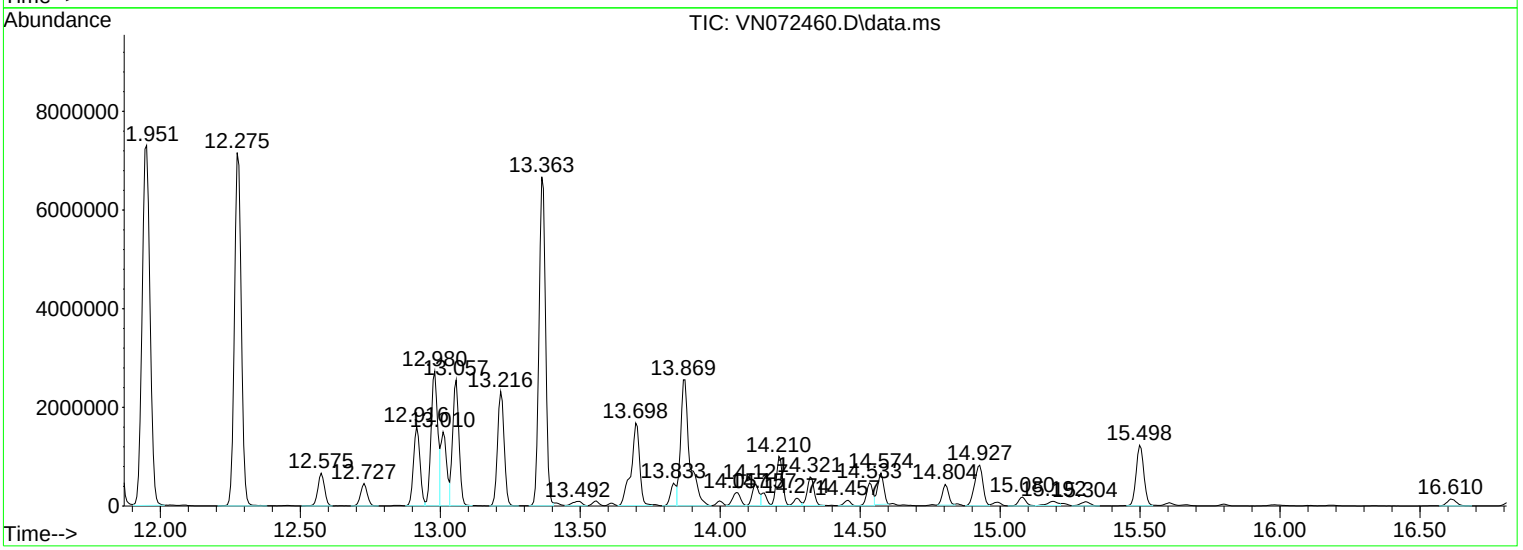
Instrument :
MSVOA_N
ClientSampleId :
GES-1

Quant Title :

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

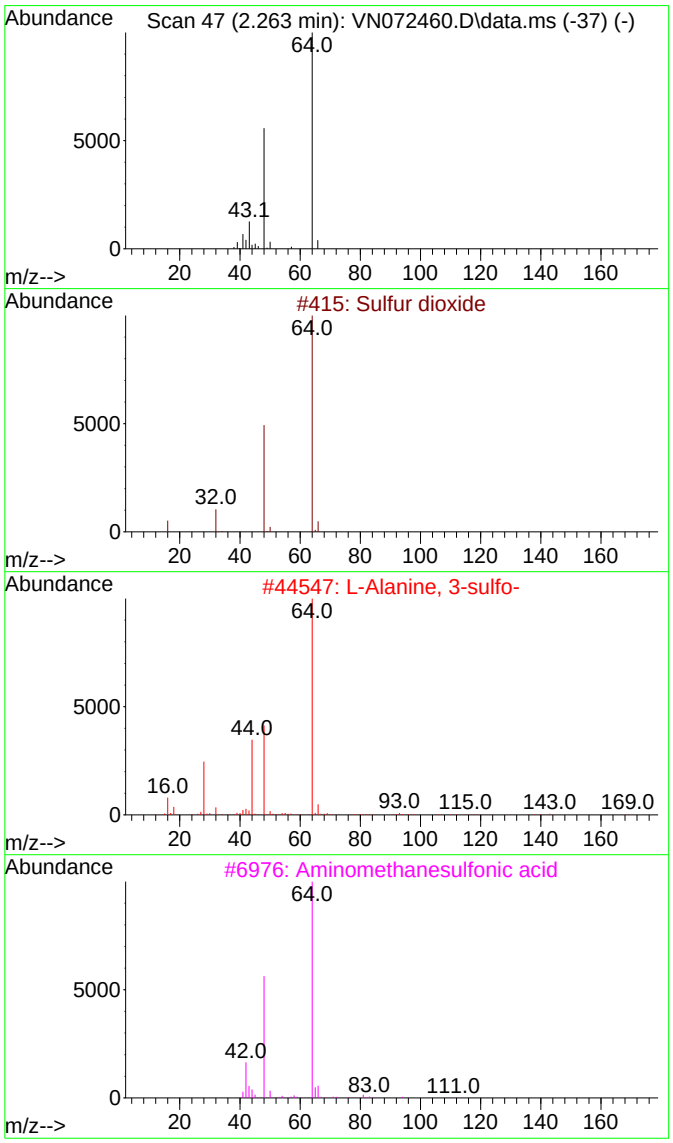
Quant Title :

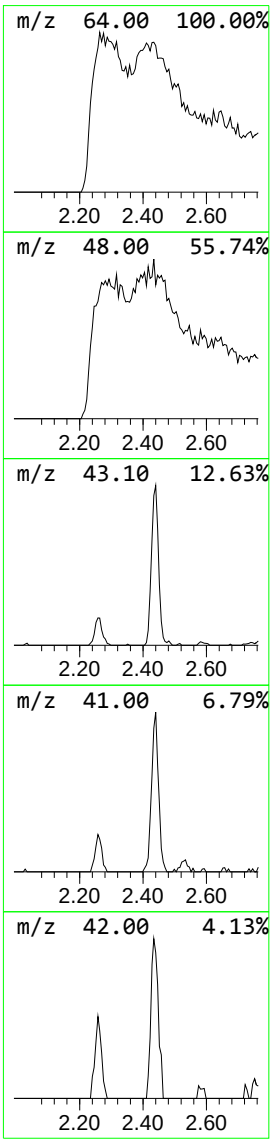
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Sulfur dioxide Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.263	13.41 ug/l	251095	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
3	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
4	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5	Ethyl Chloride	64	C2H5Cl	000075-00-3	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

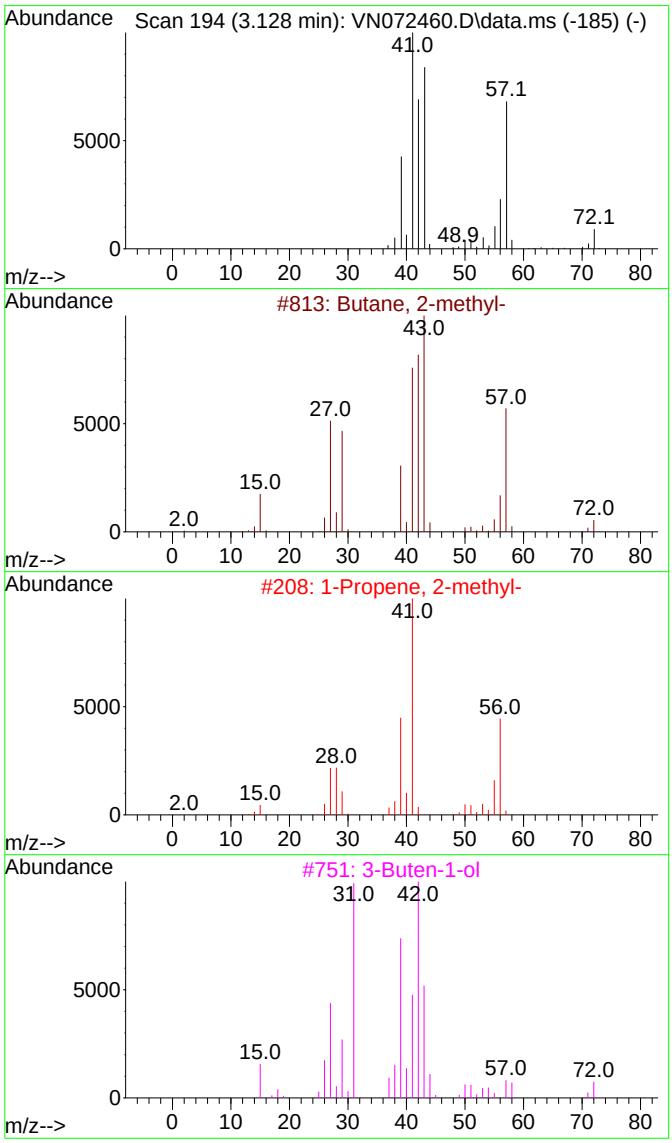
Quant Title :

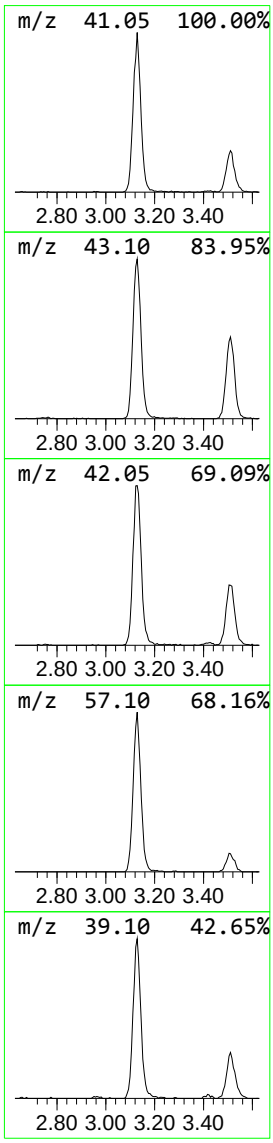
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Butane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.128	39.03 ug/l	730857	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	50
2	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
3	3-Buten-1-ol	72	C4H8O	000627-27-0	28
4	1-Butene	56	C4H8	000106-98-9	18
5	2-Butene, (E)-	56	C4H8	000624-64-6	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

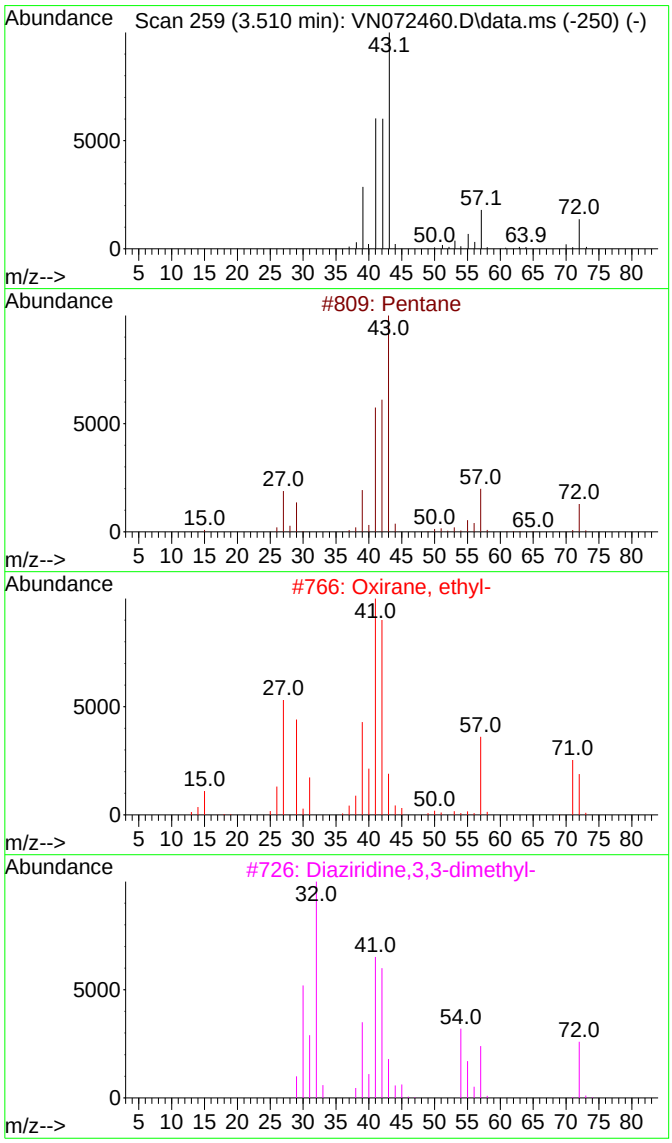
Quant Title :

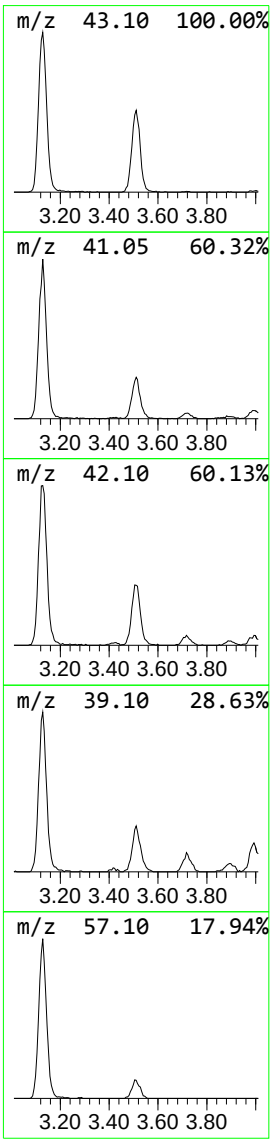
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Pentane Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.510	13.16 ug/l	246351	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane	72	C5H12	000109-66-0	90
2	Oxirane, ethyl-	72	C4H8O	000106-88-7	50
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9
4	Ethanamine, N-methylene-	57	C3H7N	043729-97-1	9
5	1-Propene, 2-methoxy-	72	C4H8O	000116-11-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

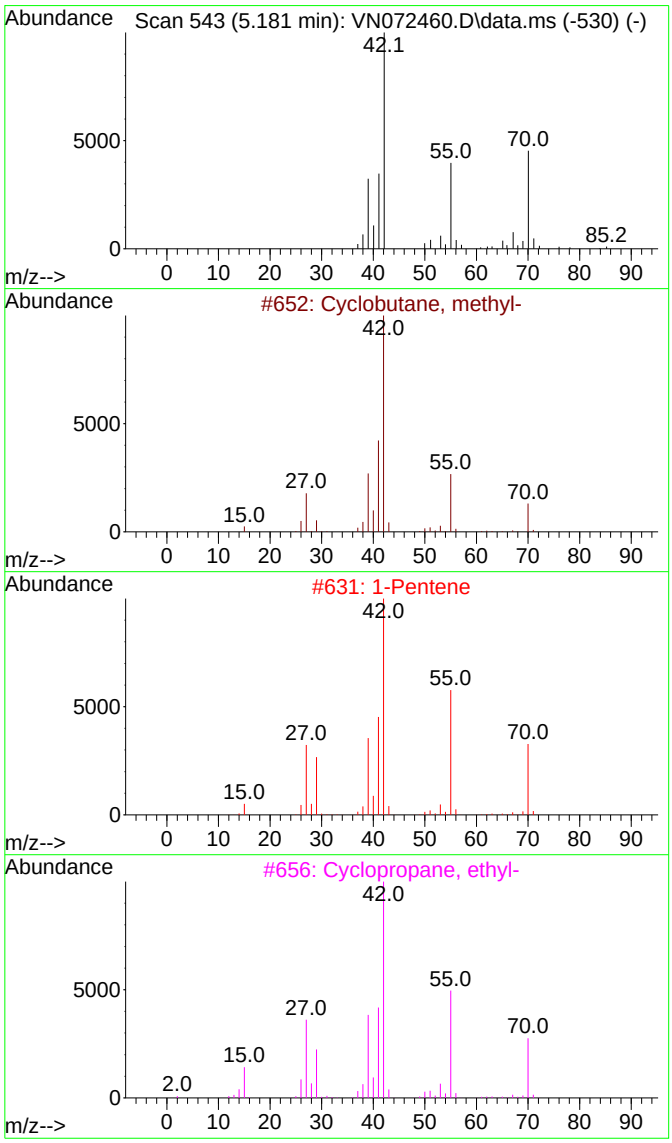
Quant Title :

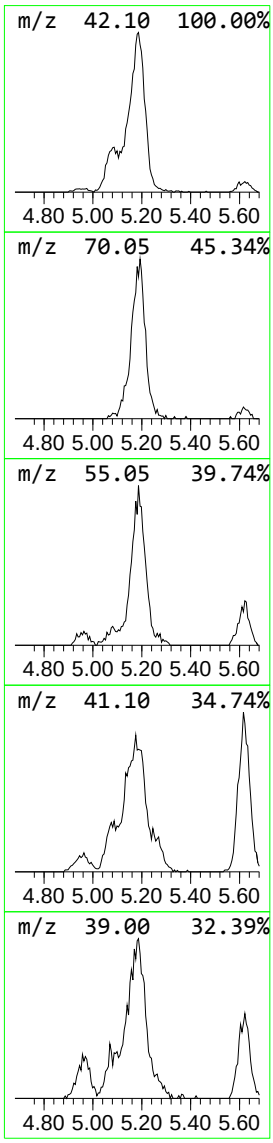
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Cyclobutane, methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.181	25.52 ug/l	477915	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, methyl-	70	C5H10	000598-61-8	72
2	1-Pentene	70	C5H10	000109-67-1	64
3	Cyclopropane, ethyl-	70	C5H10	001191-96-4	50
4	Methyl propargyl ether	70	C4H6O	000627-41-8	25
5	Isobutyronitrile	69	C4H7N	000078-82-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

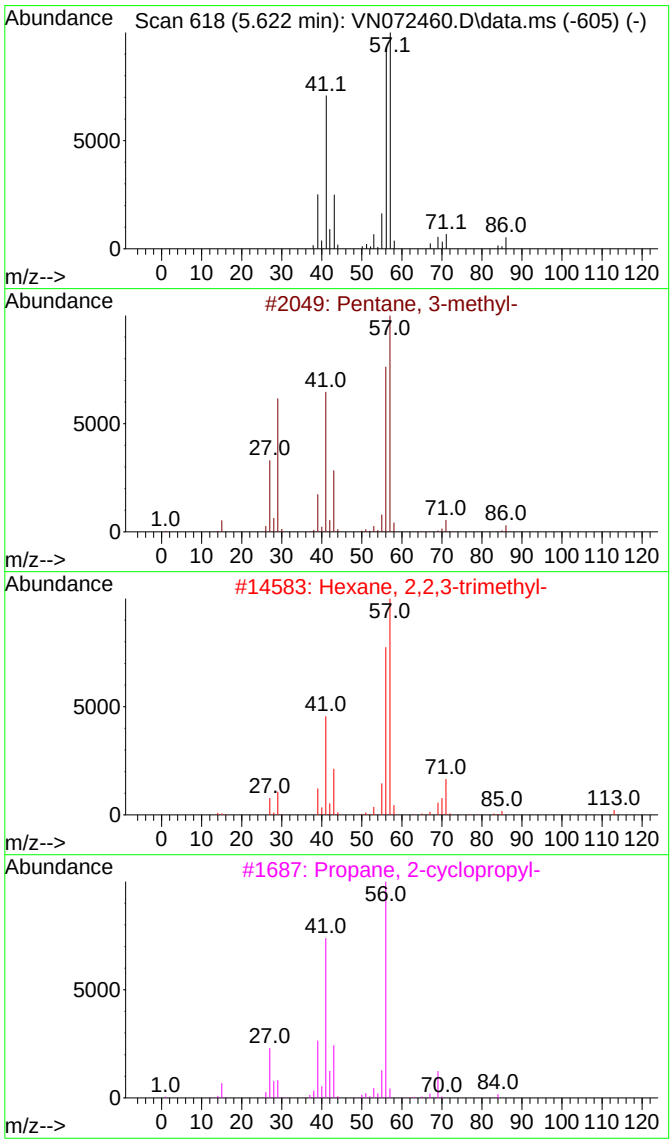
Quant Title :

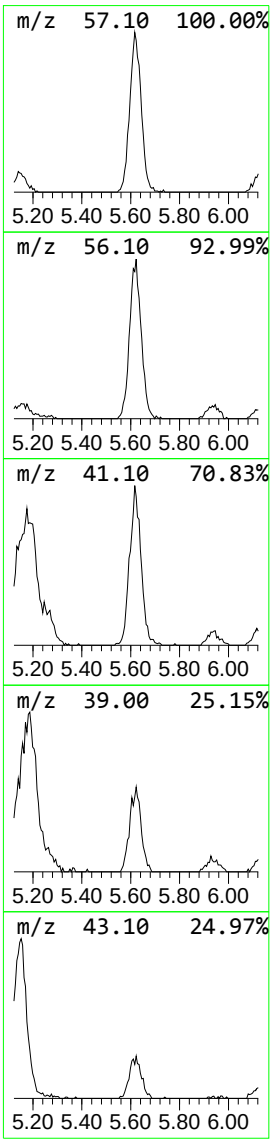
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Pentane, 3-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.622	14.94 ug/l	279803	Pentafluorobenzene	8.087

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 3-methyl-	86	C6H14	000096-14-0	86
2	Hexane, 2,2,3-trimethyl-	128	C9H20	016747-25-4	64
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	53
4	Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	45
5	Hexane, 3,4-dimethyl-	114	C8H18	000583-48-2	43





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

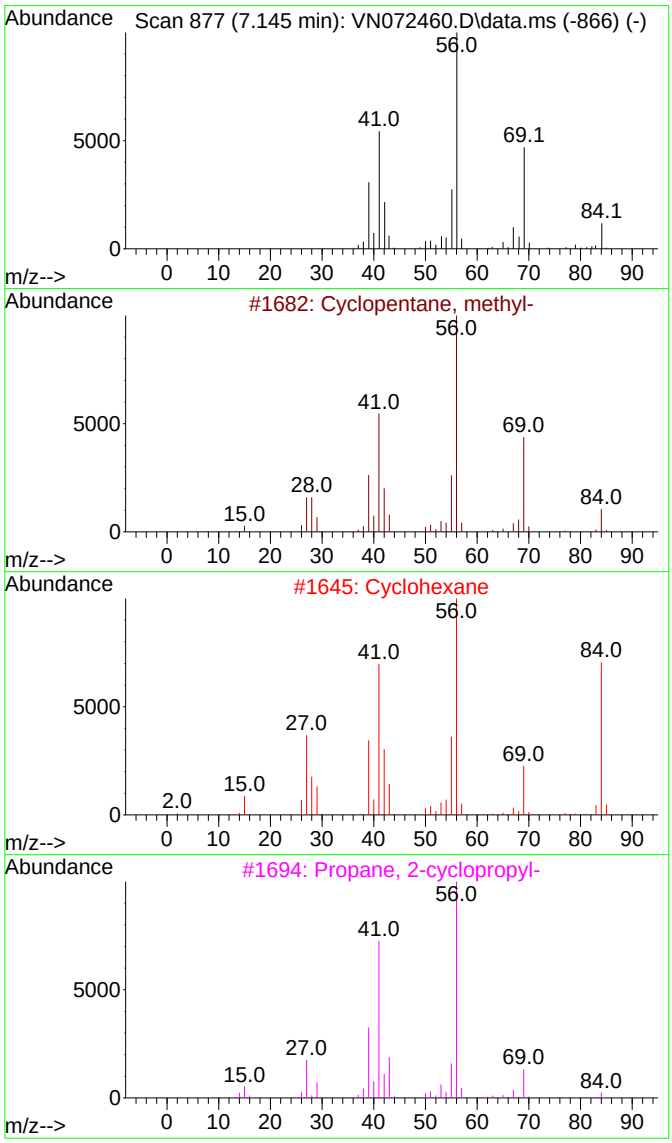
Quant Title :

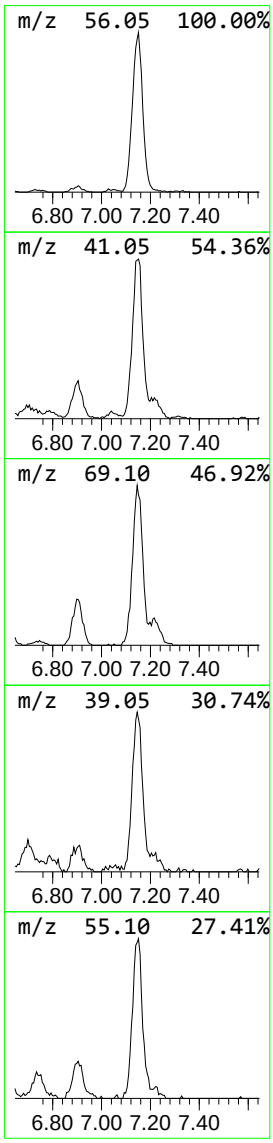
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Cyclopentane, methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.145	28.47 ug/l	533053	Pentafluorobenzene	8.087

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	87
3	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	72
4	Cyclobutane, ethyl-	84	C6H12	004806-61-5	64
5	1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

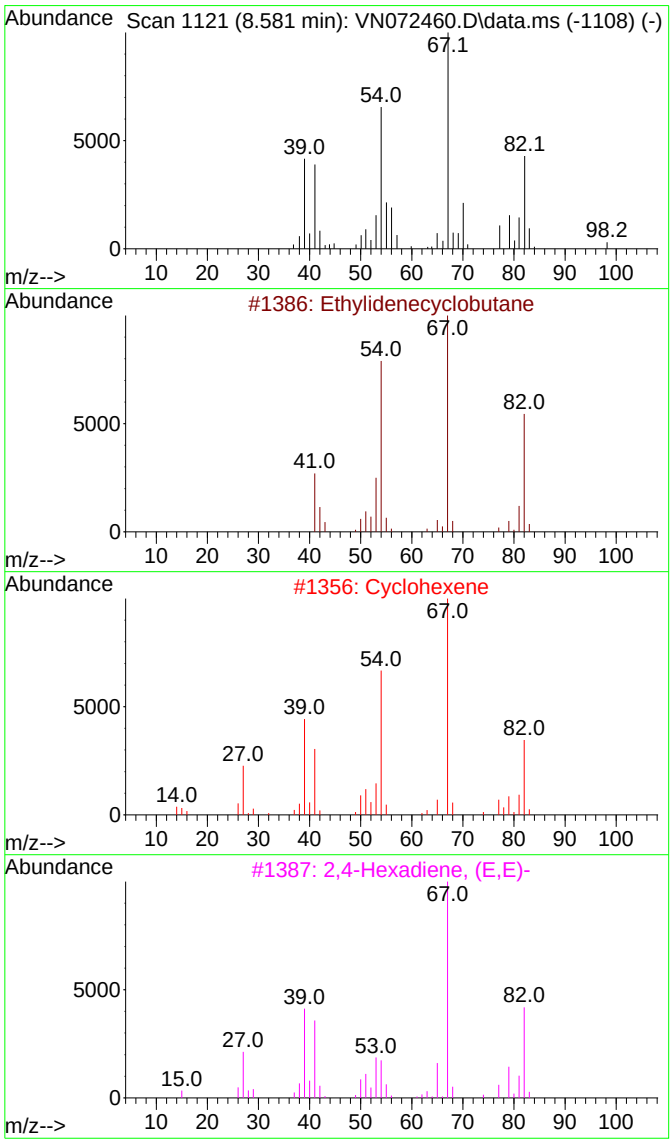
Quant Title :

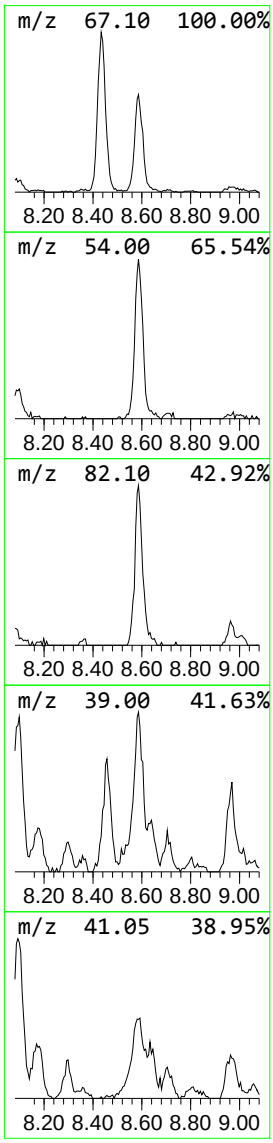
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Ethylidenecyclobutane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.581	17.23 ug/l	299146	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethylidenecyclobutane	82	C6H10	001528-21-8	76
2	Cyclohexene	82	C6H10	000110-83-8	68
3	2,4-Hexadiene, (E,E)-	82	C6H10	005194-51-4	64
4	1,3-Butadiene, 2,3-dimethyl-	82	C6H10	000513-81-5	62
5	1,3-Pentadiene, 2-methyl-, (E)-	82	C6H10	000926-54-5	58





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

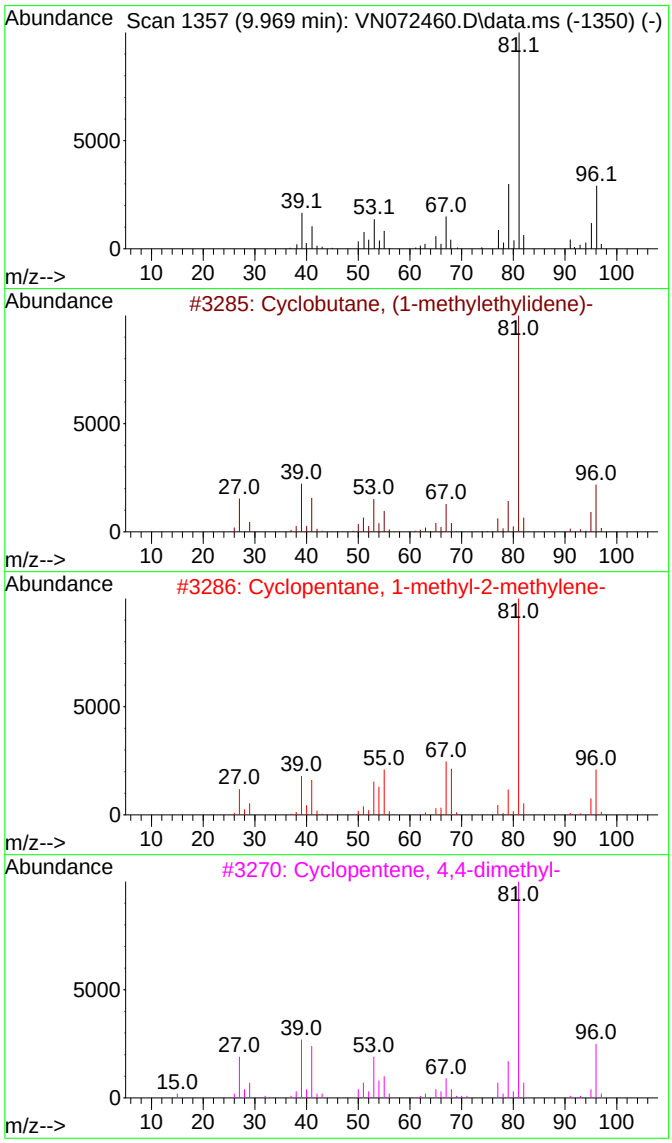
Quant Title :

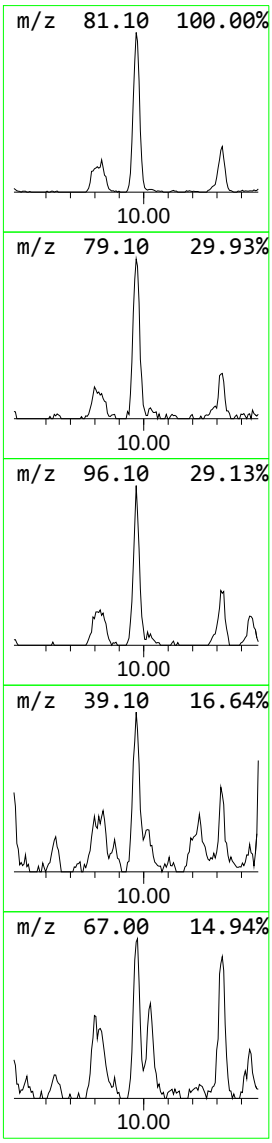
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Cyclobutane, (1-methylethyl... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.969	13.60 ug/l	236104	1,4-Difluorobenzene	8.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclobutane, (1-methylethylidene)-	96	C7H12	001528-22-9	90
2	Cyclopentane, 1-methyl-2-methylene-	96	C7H12	041158-41-2	72
3	Cyclopentene, 4,4-dimethyl-	96	C7H12	019037-72-0	72
4	(S)-2,5-Dimethyl-3-vinylhex-4-en...	154	C10H18O	035671-15-9	64
5	Cyclohexene, 4-methyl-	96	C7H12	000591-47-9	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

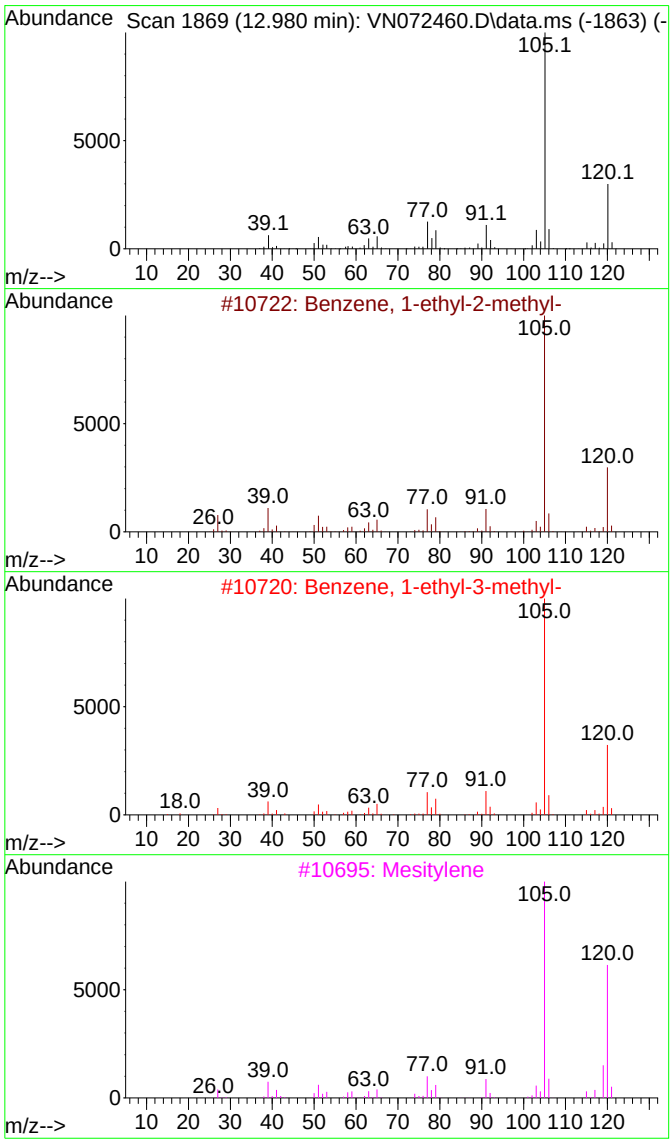
Quant Title :

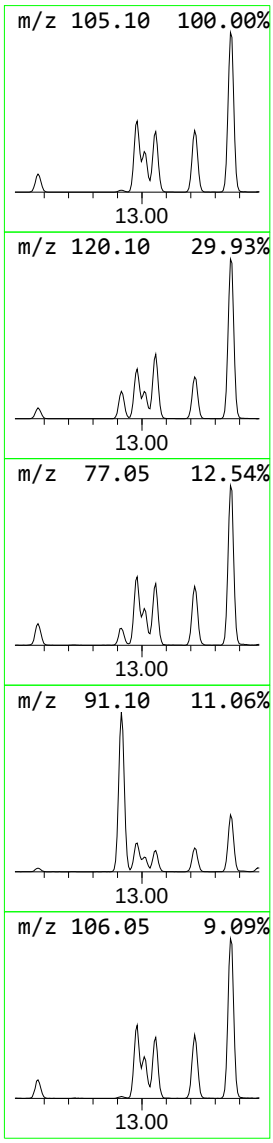
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.980	64.68 ug/l	4625310	1,4-Dichlorobenzene-d4	13.674

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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

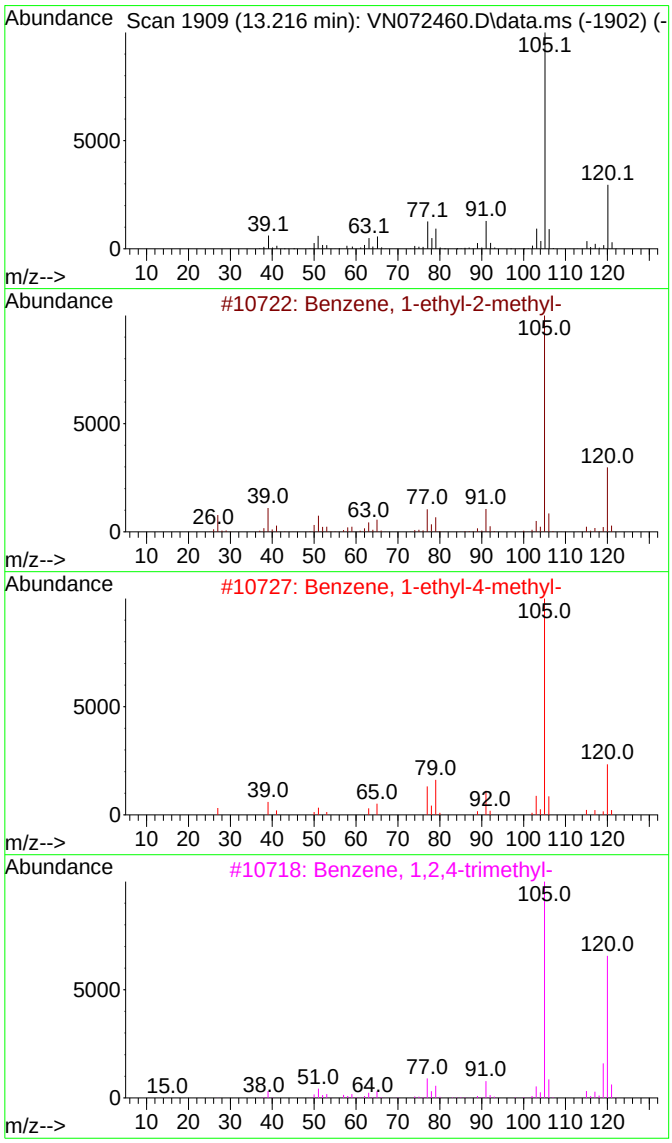
Quant Title :

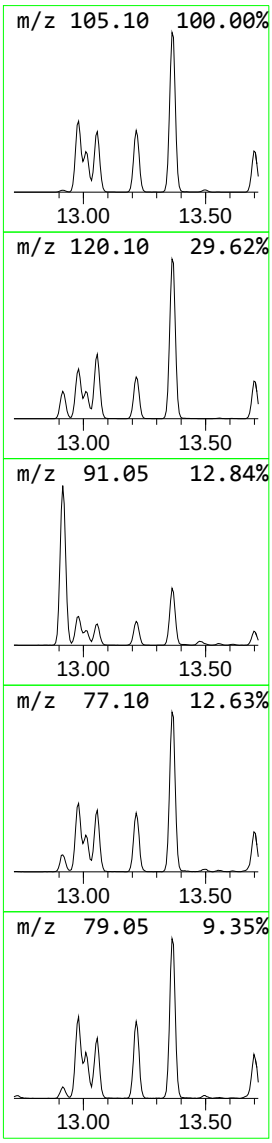
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.216	53.35 ug/l	3815110	1,4-Dichlorobenzene-d4	13.674

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	93
3	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN051222\
Data File : VN072460.D
Acq On : 12 May 2022 18:08
Operator : JC\MD
Sample : N2800-10
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
GES-1

Quant Title :

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	2.263	13.4	ug/l	251095	1	8.087	936220	50.0
Butane, 2-methyl-	3.128	39.0	ug/l	730857	1	8.087	936220	50.0
Pentane	3.510	13.2	ug/l	246351	1	8.087	936220	50.0
Cyclobutane, me...	5.181	25.5	ug/l	477915	1	8.087	936220	50.0
Pentane, 3-methyl-	5.622	14.9	ug/l	279803	1	8.087	936220	50.0
Cyclopentane, m...	7.145	28.5	ug/l	533053	1	8.087	936220	50.0
Ethylidenecyclo...	8.581	17.2	ug/l	299146	2	8.963	868046	50.0
Cyclobutane, (1...	9.969	13.6	ug/l	236104	2	8.963	868046	50.0
Benzene, 1-ethy...	12.980	64.7	ug/l	4625310	4	13.674	3575610	50.0
Benzene, 1-ethy...	13.216	53.4	ug/l	3815110	4	13.674	3575610	50.0