LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

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\82N122721W.M
Title : SW846 8260

Signal : TIC: VN070555.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.032	7	16	36	rVB	546222	815068	7.72%	1.085%
2	2.247	85	96	116	rVB4	98528	254815	2.41%	0.339%
3	2.421	150	161	166	rBV	200456	322980	3.06%	0.430%
4	2.593	209	225	264	rBV	4154195	7596973	71.98%	10.116%
5	3.693	615	635	657	rVB2	191650	563296	5.34%	0.750%
6	4.146	779	804	835	rBV	713794	2041938	19.35%	2.719%
7	4.288	836	857	903	rVB	733673	2176331	20.62%	2.898%
8	4.588	946	969	997	rBV2	115551	373279	3.54%	0.497%
9	5.398	1241	1271	1297	rBV6	34612	144574	1.37%	0.193%
10	5.967	1460	1483	1504	rBV2	37425	119655	1.13%	0.159%
11	6.493	1652	1679	1691	rBV5	50460	170528	1.62%	0.227%
12	6.586	1692	1714	1767	rVB2	1026897	3382123	32.05%	4.504%
13	7.064	1864	1892	1910	rBV2	517555	1538325	14.58%	2.048%
14	7.150	1911	1924	1961	rVB2	380667	1064466	10.09%	1.417%
15	7.337	1977	1994	2023	rVB2	86240	236641	2.24%	0.315%
16	8.021	2226	2249	2259	rBV	731024	1710809	16.21%	2.278%
17	8.086	2260	2273	2296	rVB	1567005	3581139	33.93%	4.769%
18	8.434	2379	2403	2428	rBV2	905790	2335178	22.13%	3.109%
19	8.839	2536	2554	2572	rVB6	51396	128250	1.22%	0.171%
20	8.968	2582	2602	2635	rBV	2597021	5479492	51.92%	7.296%
21	9.158	2655	2673	2707	rBV	992461	2484582	23.54%	3.308%
22	9.531	2798	2812	2839	rVB3	74403	176592	1.67%	0.235%
23	10.271	3060	3088	3090	rBV6	40057	123104	1.17%	0.164%
24	10.440	3132	3151	3165	rBV	3435910	6520865	61.79%	8.683%
25	10.502	3165	3174	3195	rVB	756382	1377365	13.05%	1.834%
26	10.682	3225	3241	3263	rVB4	108866	249700	2.37%	0.332%
27	10.856	3285	3306	3327	rBV3	120256	299721	2.84%	0.399%
28	11.135	3376	3410	3463	rBV	2848325	10554075	100.00%	14.054%
29	11.741	3615	3636	3660	rVB	2250674	4299603	40.74%	5.725%
30	11.851	3662	3677	3693	rBV4	187192	466733	4.42%	0.621%
31	11.948	3699	3713	3738	rVB	591797	1238543	11.74%	1.649%
32	12.278	3824	3836	3864	rVB	304433	608377	5.76%	0.810%
33	12.575	3933	3947	3962	rBV4	64408	130649	1.24%	0.174%
34	12.728	3990	4004	4031	rVB	1359537	2374912	22.50%	3.162%
35	12.983	4086	4099	4103	rBV2	80909	132803	1.26%	0.177%
36	13.047	4116	4123	4142	rVB7	117775	223481	2.12%	0.298%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

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\82N122721W.M
Title : SW846 8260

37	13.160	4149	4165	4180	rBV3	1124338	2183195	20.69%	2.907%
38	13.227	4182	4190	4206	rVB	432419	741619	7.03%	0.988%
39	13.366	4233	4242	4253	rBV2	124848	202214	1.92%	0.269%
40	13.578	4309	4321	4340	rVB5	200399	384981	3.65%	0.513%
41	13.672	4341	4356	4378	rBV	1047877	1956027	18.53%	2.605%
42	13.766	4381	4391	4408	rVB	226188	384098	3.64%	0.511%
43	13.991	4466	4475	4485	rBV6	65807	114635	1.09%	0.153%
44	14.053	4488	4498	4511	rVV3	169858	304361	2.88%	0.405%
45	14.117	4511	4522	4546	rVV4	212354	511079	4.84%	0.681%
46	14.211	4550	4557	4568	rVB3	79272	126314	1.20%	0.168%
47	14.490	4651	4661	4675	rVV3	350638	648429	6.14%	0.863%
48	14.844	4786	4793	4806	rVB3	169902	270047	2.56%	0.360%
49	14.922	4808	4822	4833	rBV6	165315	424423	4.02%	0.565%
50	15.196	4916	4924	4929	rBV5	76516	117787	1.12%	0.157%
51	15.300	4956	4963	4977	rVB7	98383	169293	1.60%	0.225%
52	16.019	5221	5231	5251	rVB2	327956	610062	5.78%	0.812%
53	16.319	5332	5343	5361	rVB2	307216	652781	6.19%	0.869%

Sum of corrected areas: 75098310

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
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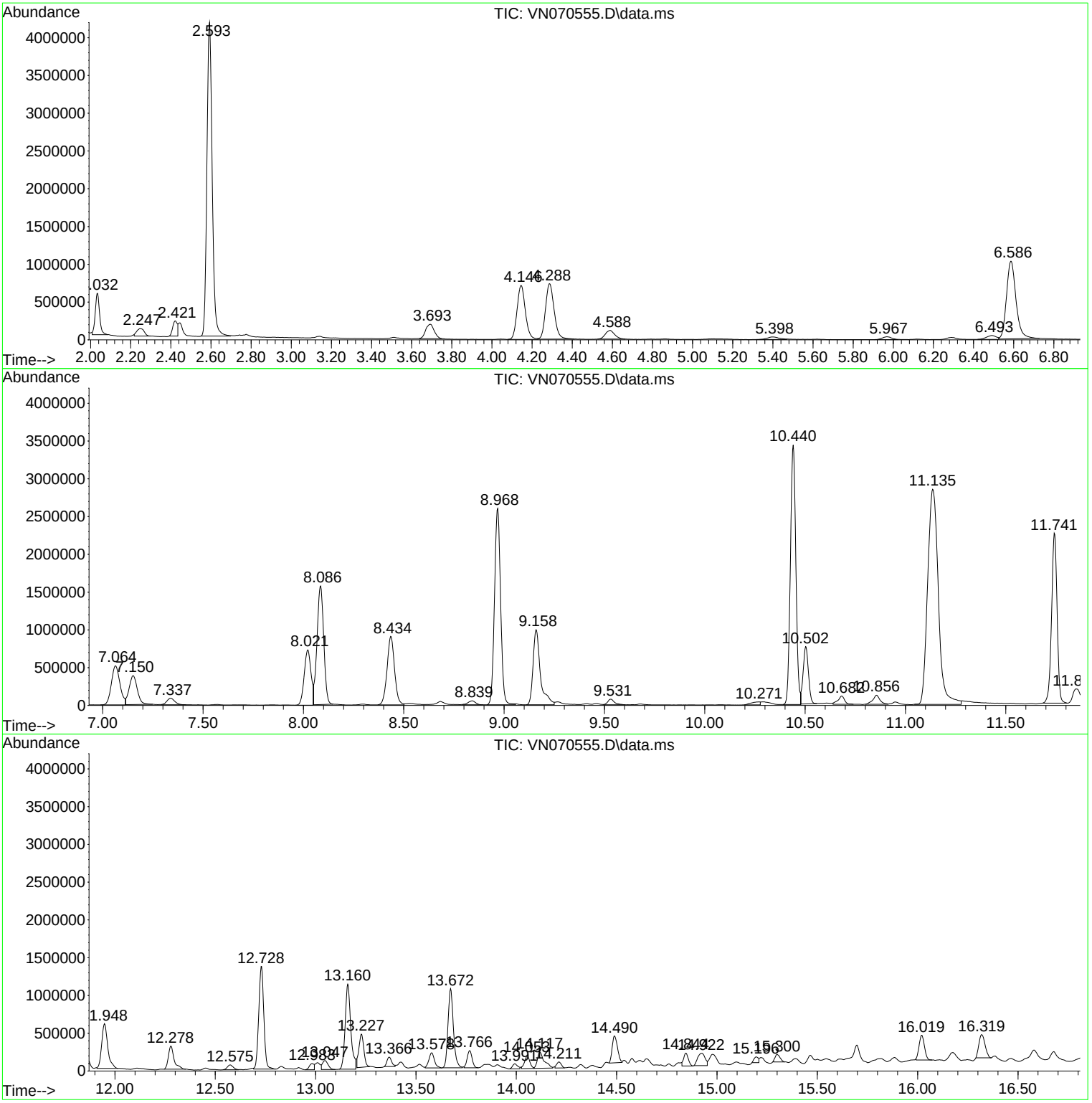
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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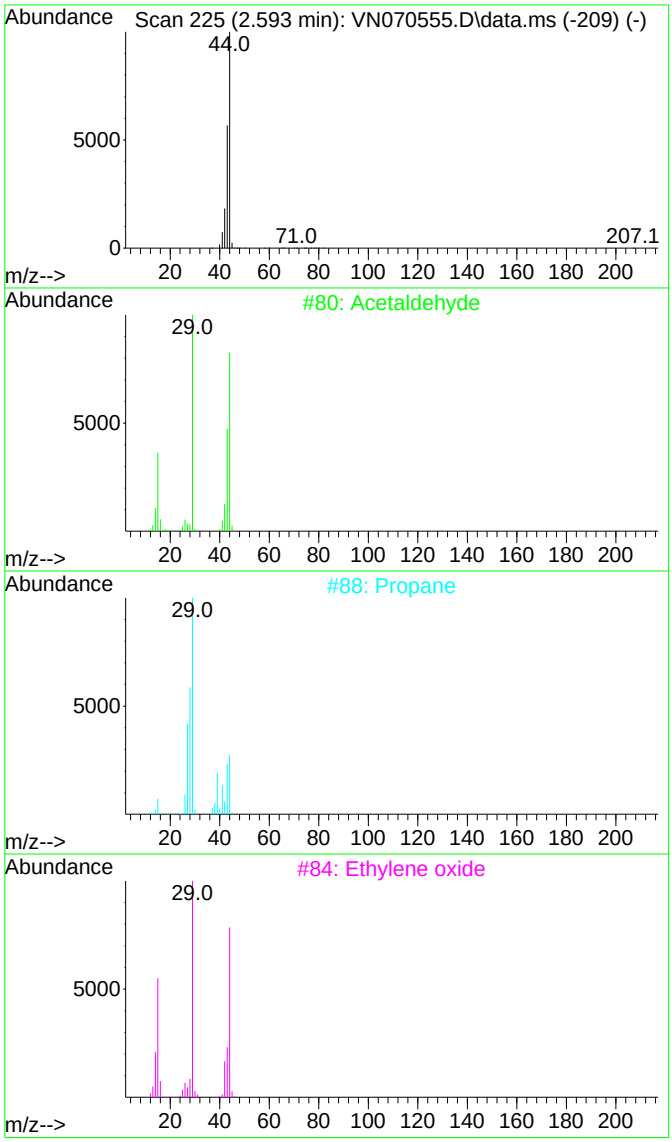
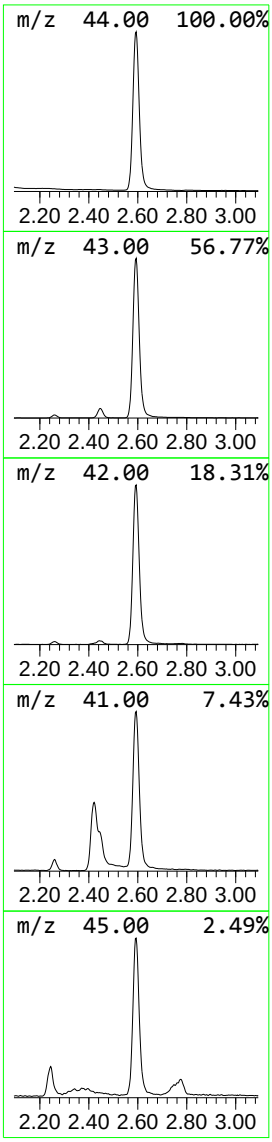
Peak Number 1 unknown2.593 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.593	106.07 ug/l	7596970	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	9
2	Propane	44	C3H8	000074-98-6	5
3	Ethylene oxide	44	C2H4O	000075-21-8	5
4	Alanine	89	C3H7NO2	000056-41-7	4
5	Hydrogen isocyanate	43	CHNO	000075-13-8	3





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

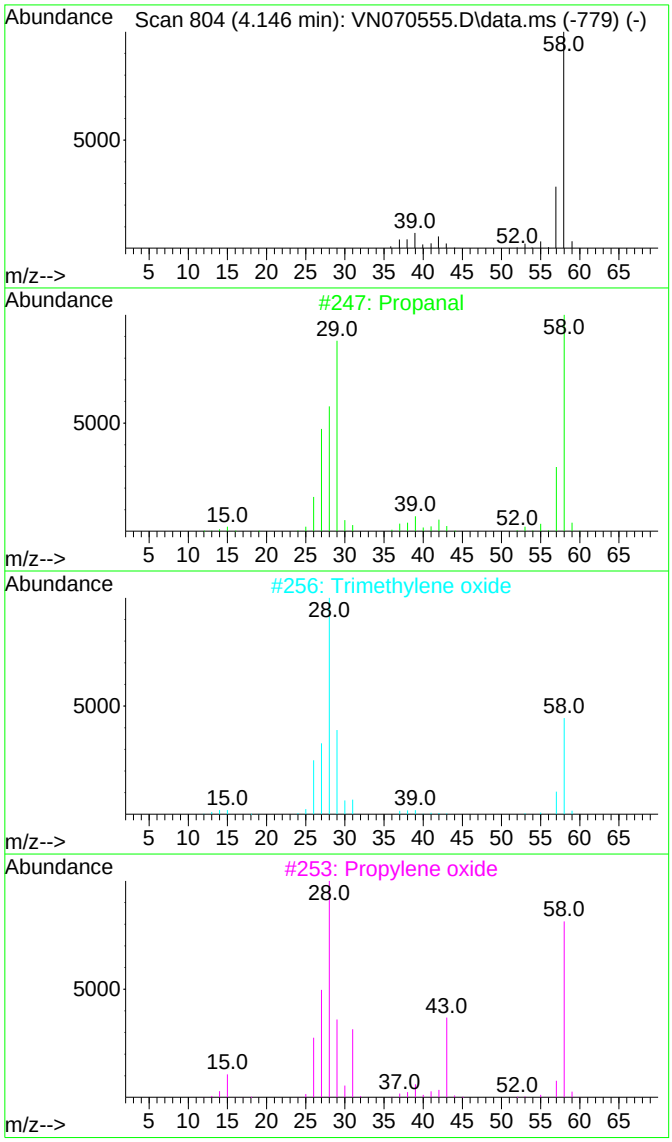
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

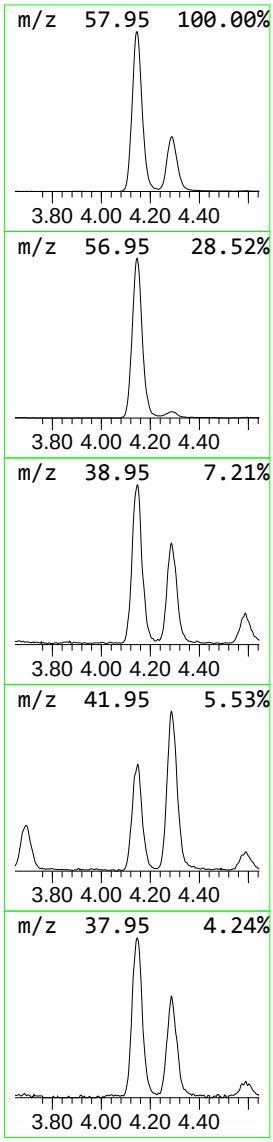
****

Peak Number 2 Propanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.146	28.51 ug/l	2041940	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	78
2	Trimethylene oxide	58	C3H6O	000503-30-0	9
3	Propylene oxide	58	C3H6O	000075-56-9	7
4	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	5
5	Borane, compd. with dimethylamin...	59	C2H10BN	000074-94-2	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

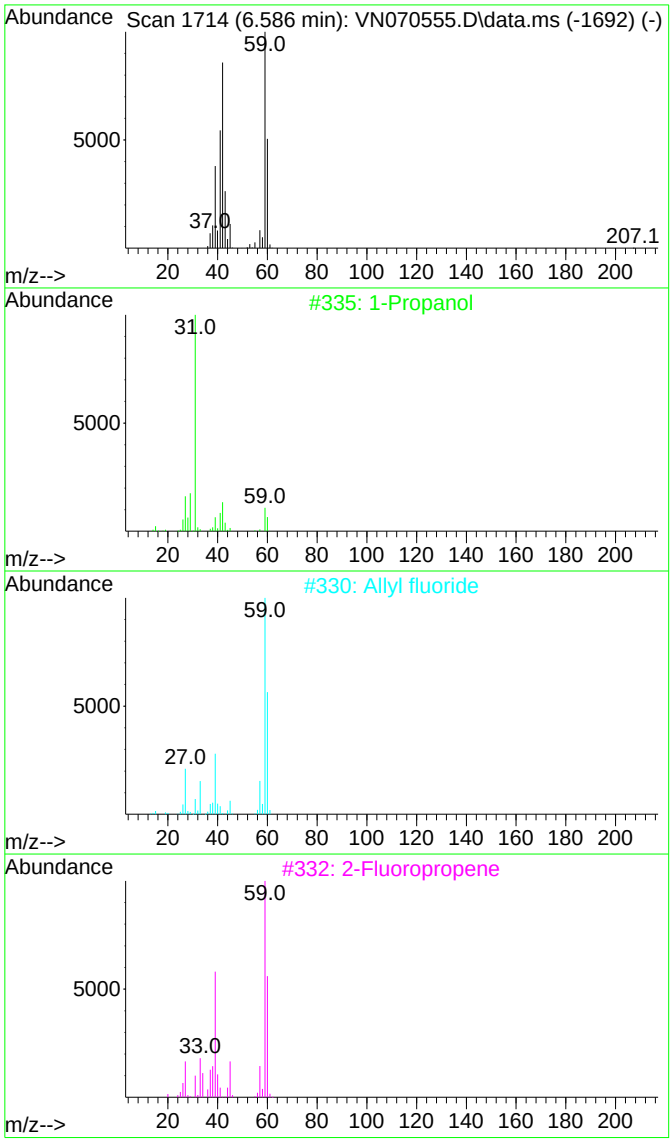
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

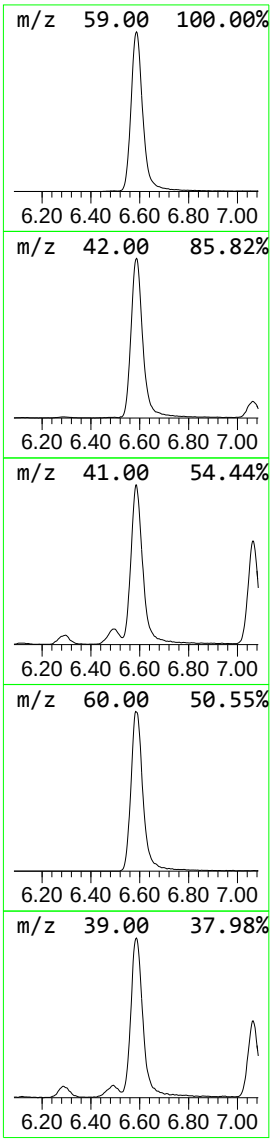
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1-Propanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.586	47.22 ug/l	3382120	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	Allyl fluoride	60	C3H5F	000818-92-8	47
3	2-Fluoropropene	60	C3H5F	001184-60-7	37
4	2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	12
5	Cyclopropane	42	C3H6	000075-19-4	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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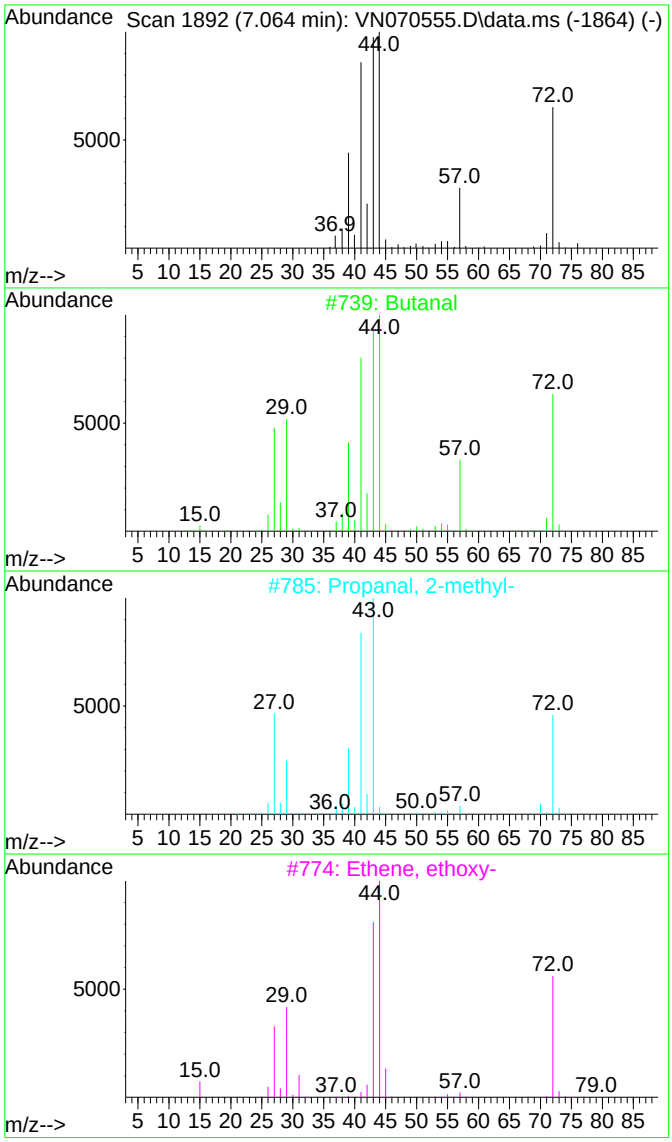
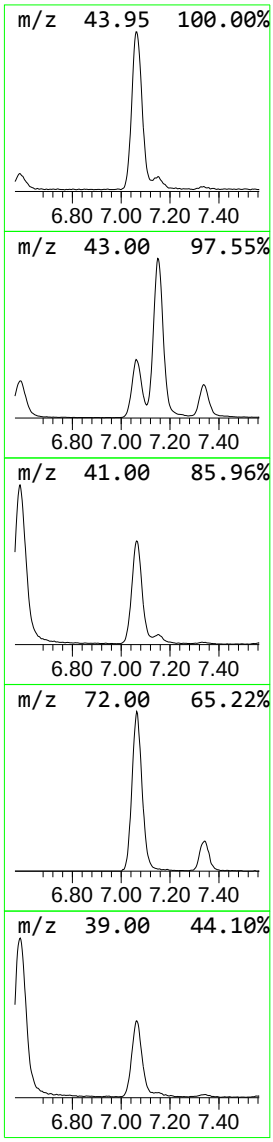
Peak Number 4 Butanal Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.064	21.48 ug/l	1538330	Pentafluorobenzene	8.086

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	Propanal, 2-methyl-	72	C4H8O	000078-84-2	49
3	Ethene, ethoxy-	72	C4H8O	000109-92-2	47
4	O-Methylisourea	74	C2H6N2O	002440-60-0	42
5	2-Propanone, hydrazone	72	C3H8N2	005281-20-9	27





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

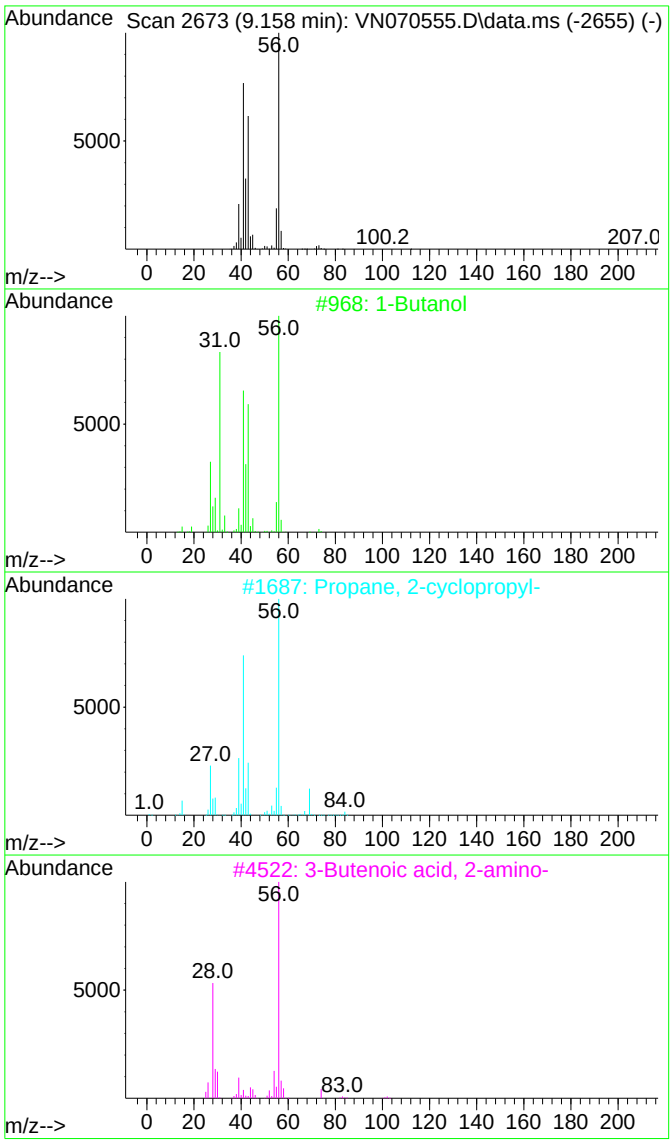
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

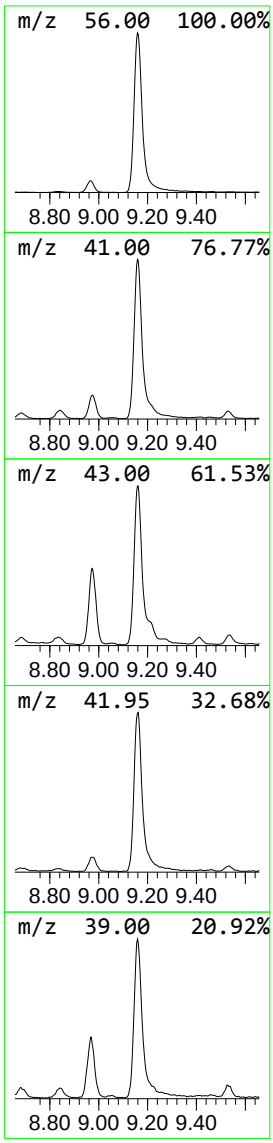
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 1-Butanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.158	22.67 ug/l	2484580	1,4-Difluorobenzene	8.965

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	91
2	Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	39
3	3-Butenoic acid, 2-amino-	101	C4H7NO2	056512-51-7	9
4	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9
5	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
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20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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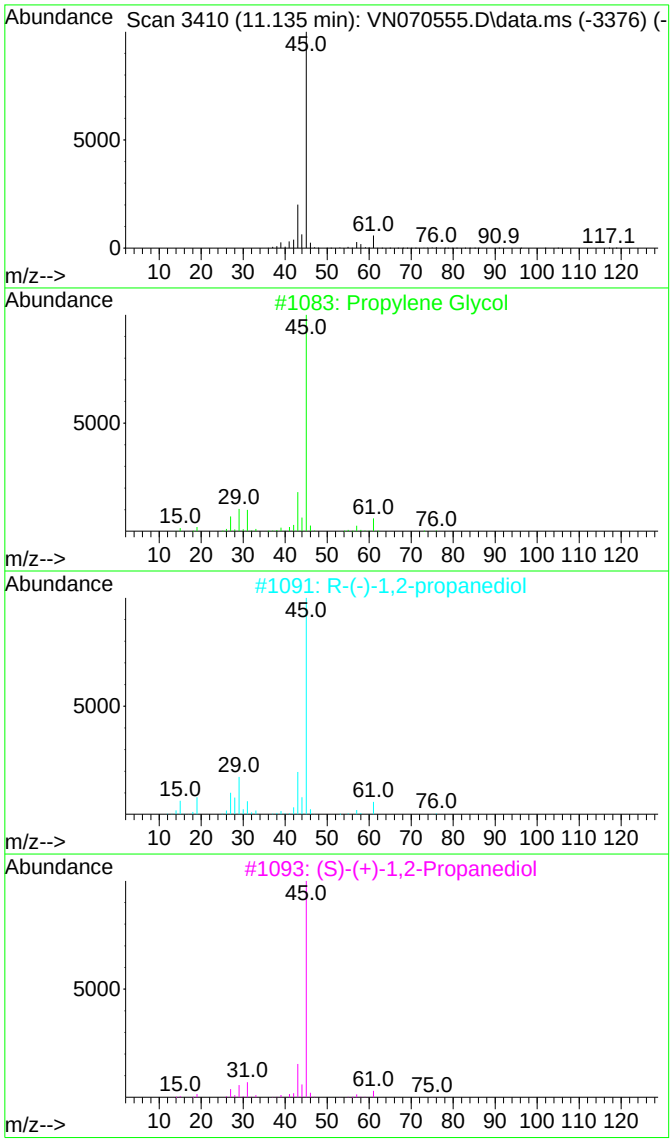
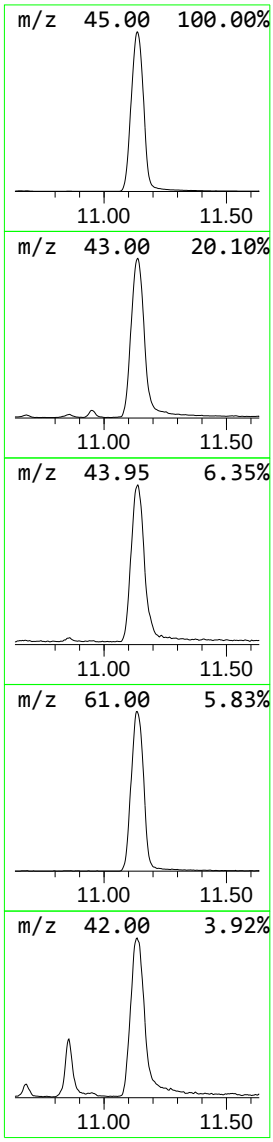
Peak Number 6 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.135	122.73 ug/l	10554100	Chlorobenzene-d5	11.744

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	78
3	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	56
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
5	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40





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Data File : VN070555.D
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Operator : JC/MD
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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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

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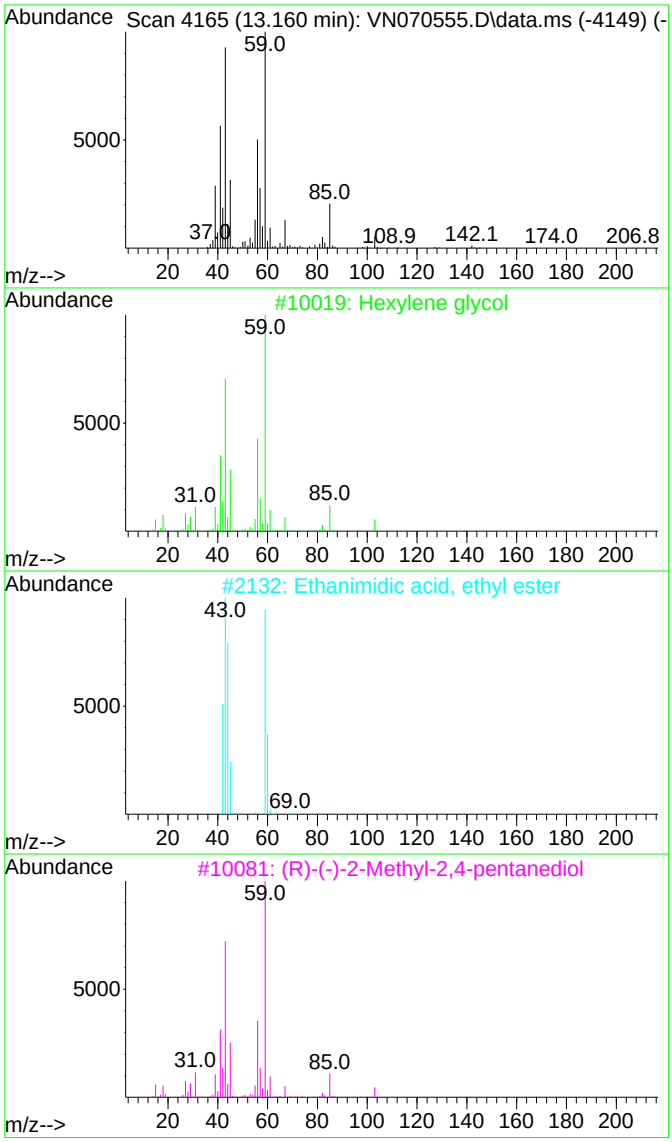
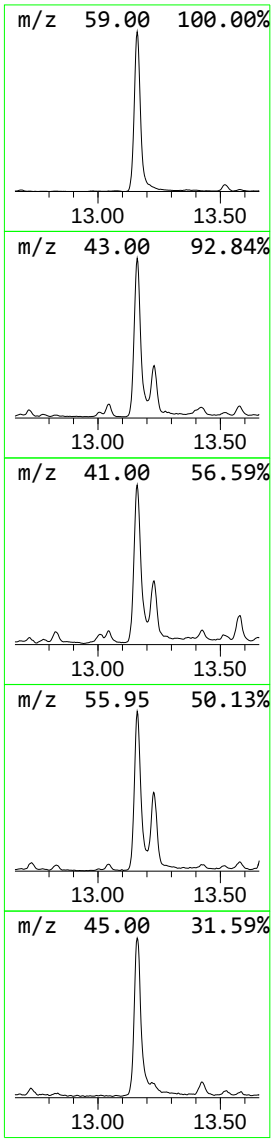
Peak Number 7 Hexylene glycol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.160	55.81 ug/l	2183200	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexylene glycol	118	C6H14O2	000107-41-5	64
2	Ethanimidic acid, ethyl ester	87	C4H9NO	001000-84-6	43
3	(R)-(-)-2-Methyl-2,4-pentanediol	118	C6H14O2	099210-90-9	42
4	2,4-Dimethyl-2,4-pentanediol	132	C7H16O2	024892-49-7	40
5	Acetic acid, ethoxy-, 1-methylet...	146	C7H14O3	054063-13-7	40





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Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

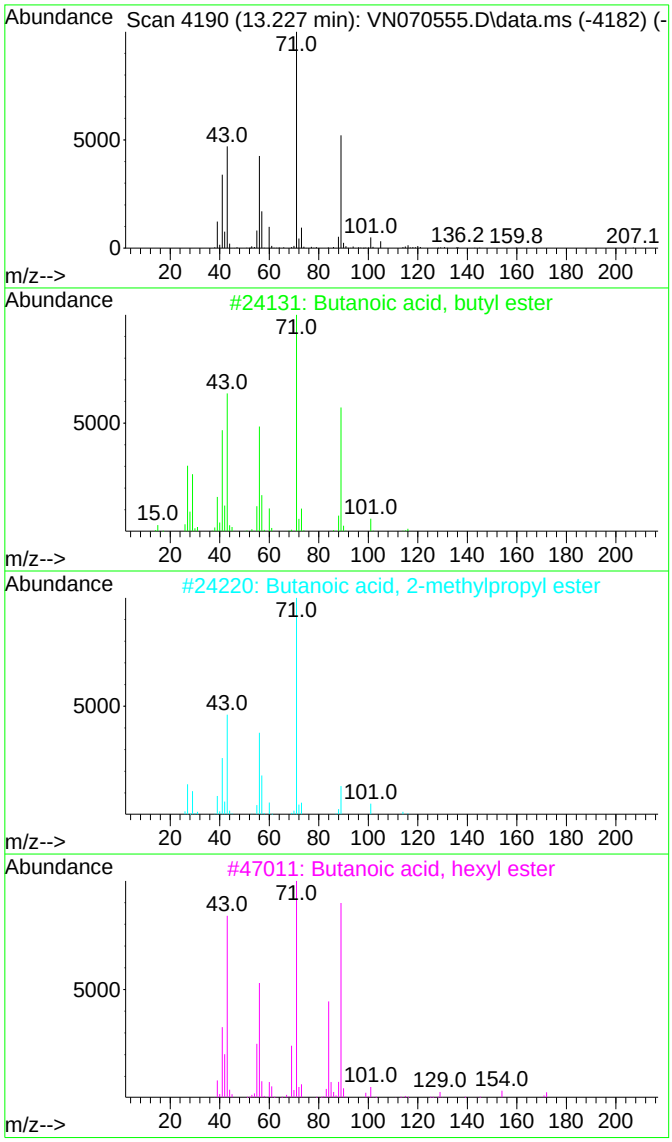
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

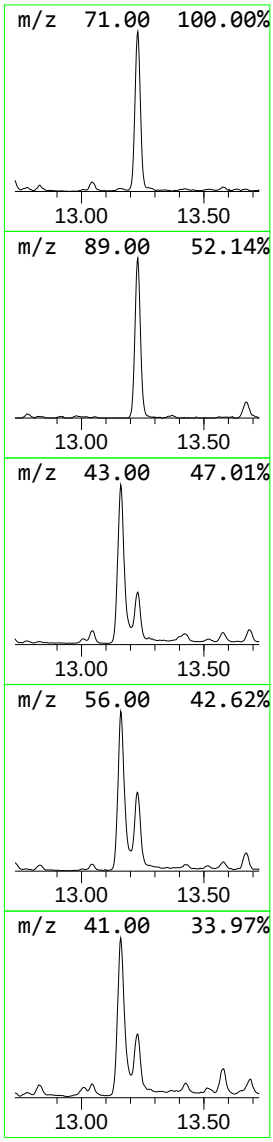
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Butanoic acid, butyl ester Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.227	18.96 ug/l	741619	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanoic acid, butyl ester	144	C8H16O2	000109-21-7	72
2	Butanoic acid, 2-methylpropyl ester	144	C8H16O2	000539-90-2	72
3	Butanoic acid, hexyl ester	172	C10H20O2	002639-63-6	64
4	Propanoic acid, 2-methyl-, 2-met...	144	C8H16O2	000097-85-8	59
5	Propanoic acid, 2-methyl-, 2-eth...	216	C12H24O3	074367-31-0	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

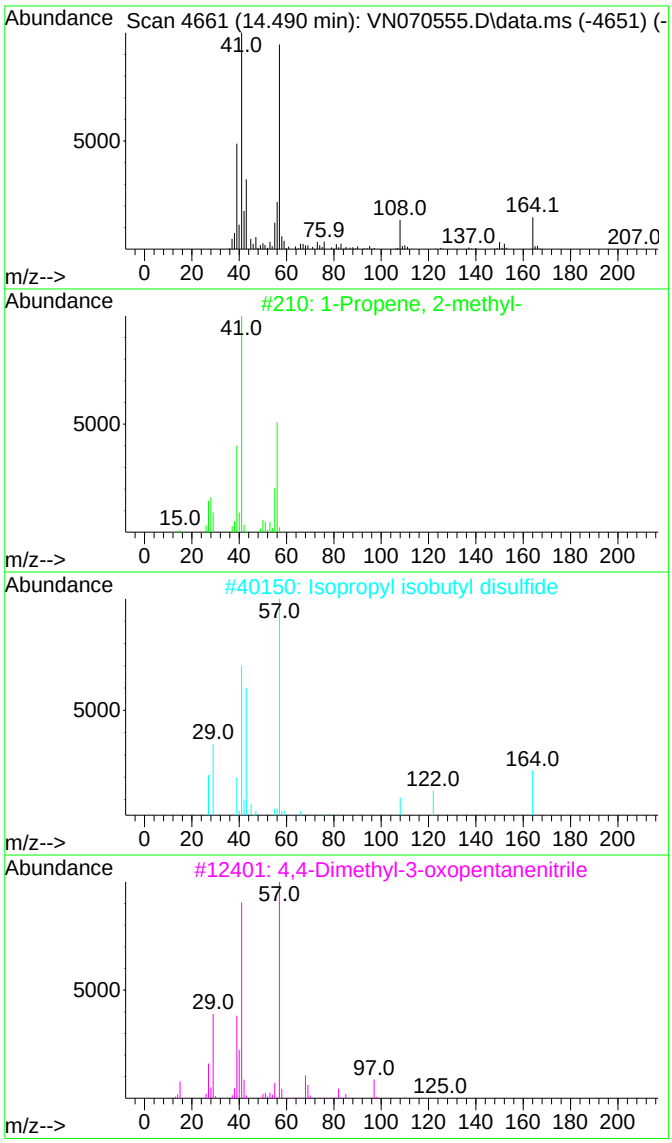
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

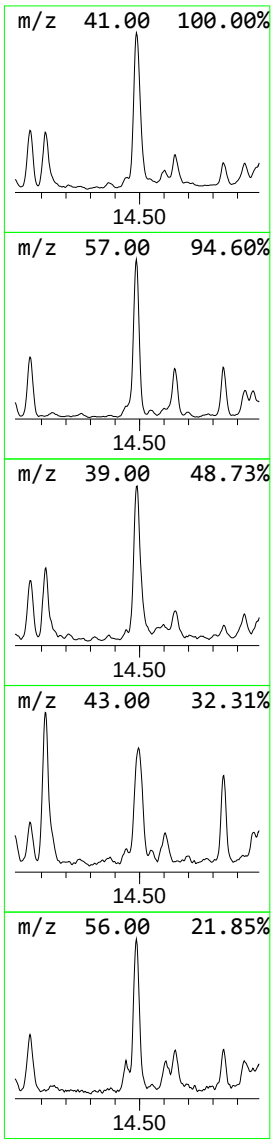
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 unknown14.490 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.490	16.58 ug/l	648429	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	43
2	Isopropyl isobutyl disulfide	164	C7H16S2	067421-82-3	35
3	4,4-Dimethyl-3-oxopentanenitrile	125	C7H11NO	059997-51-2	32
4	Ethenyl tert-butyl sulfoxide	132	C6H12OS	042779-15-7	32
5	Nitroxide, bis(1,1-dimethylethyl)	144	C8H18NO	002406-25-9	28





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

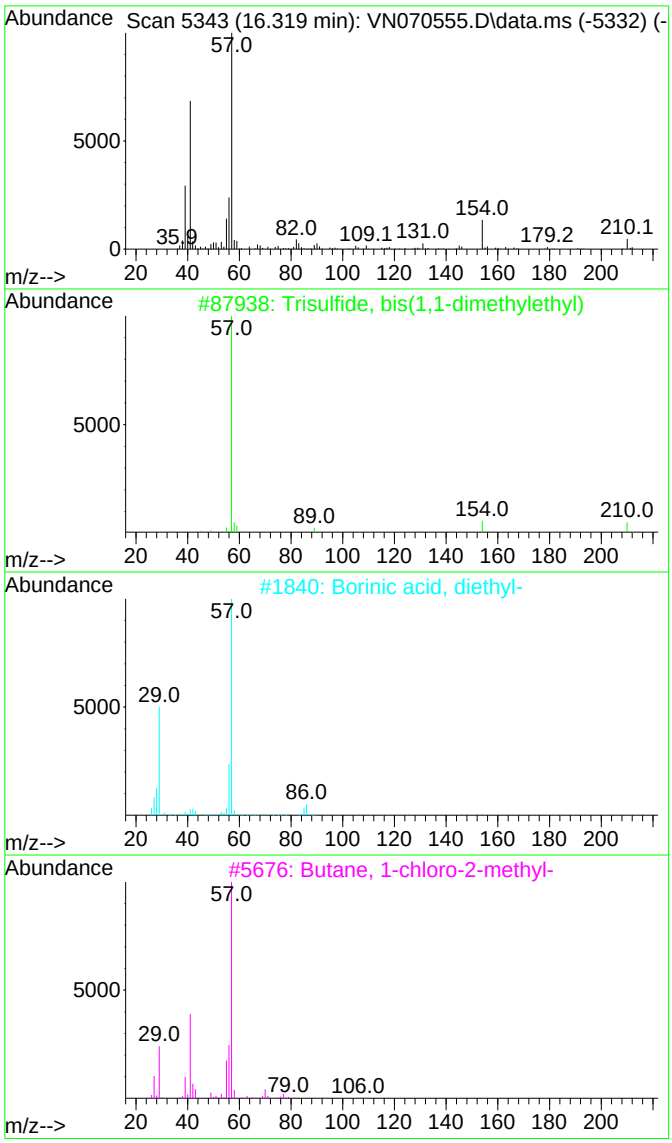
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

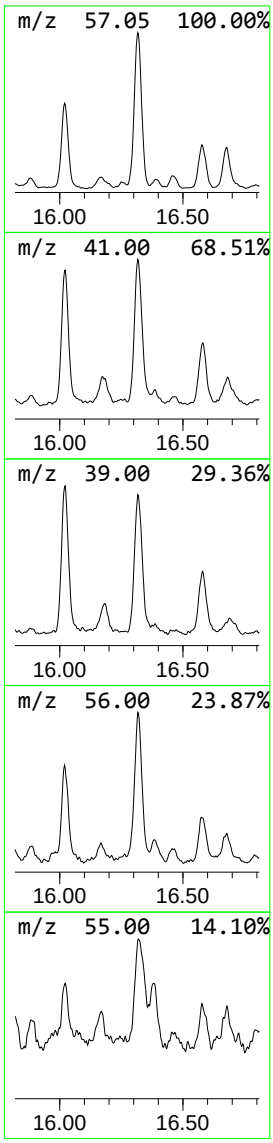
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 unknown16.319 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.319	16.69 ug/l	652781	1,4-Dichlorobenzene-d4	13.672

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	46
2	Borinic acid, diethyl-	86	C4H11BO	004426-31-7	43
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	25
4	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	25
5	Ethanedioic acid, dibutyl ester	202	C10H18O4	002050-60-4	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011022\
Data File : VN070555.D
Acq On : 10 Jan 2022 20:16
Operator : JC/MD
Sample : N1015-06
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
20985

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.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
unknown2.593	2.593	106.1	ug/l	7596970	1	8.086	3581140	50.0
Propanal	4.146	28.5	ug/l	2041940	1	8.086	3581140	50.0
1-Propanol	6.586	47.2	ug/l	3382120	1	8.086	3581140	50.0
Butanal	7.064	21.5	ug/l	1538330	1	8.086	3581140	50.0
1-Butanol	9.158	22.7	ug/l	2484580	2	8.965	5479490	50.0
Propylene Glycol	11.135	122.7	ug/l	10554100	3	11.744	4299600	50.0
Hexylene glycol	13.160	55.8	ug/l	2183200	4	13.672	1956030	50.0
Butanoic acid, ...	13.227	19.0	ug/l	741619	4	13.672	1956030	50.0
unknown14.490	14.490	16.6	ug/l	648429	4	13.672	1956030	50.0
unknown16.319	16.319	16.7	ug/l	652781	4	13.672	1956030	50.0