LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

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\82N122220W.M
Title : SW846 8260

Signal : TIC: VN065463.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	162	176	200	rBV	759533	1288058	39.51%	6.821%
2	3.261	455	473	500	rBV	128827	325758	9.99%	1.725%
3	3.669	584	600	618	rBV	54816	141522	4.34%	0.749%
4	3.791	623	638	662	rVB	87436	230365	7.07%	1.220%
5	4.055	692	720	742	rVB	60524	186210	5.71%	0.986%
6	4.296	776	795	817	rBV	83843	235867	7.24%	1.249%
7	5.377	1111	1131	1153	rVB3	18234	60622	1.86%	0.321%
8	6.032	1310	1335	1384	rBV	1020563	3259674	100.00%	17.262%
9	6.508	1462	1483	1501	rBV2	64682	195730	6.00%	1.037%
10	6.611	1501	1515	1545	rVB2	28486	87748	2.69%	0.465%
11	7.553	1790	1808	1819	rBV	140803	346081	10.62%	1.833%
12	7.630	1820	1832	1865	rVB	235204	562639	17.26%	2.980%
13	7.991	1927	1944	1977	rBV2	183083	440121	13.50%	2.331%
14	8.254	2011	2026	2045	rBV2	37171	87455	2.68%	0.463%
15	8.421	2065	2078	2096	rBV3	21778	48382	1.48%	0.256%
16	8.560	2103	2121	2157	rBV3	819507	1838979	56.42%	9.739%
17	8.765	2170	2185	2193	rBV	149547	314795	9.66%	1.667%
18	8.810	2194	2199	2212	rVB2	83736	145615	4.47%	0.771%
19	10.061	2571	2588	2602	rBV	607101	1143819	35.09%	6.057%
20	10.322	2657	2669	2694	rVB2	77579	143897	4.41%	0.762%
21	10.502	2719	2725	2747	rVV3	31398	66630	2.04%	0.353%
22	10.788	2790	2814	2886	rBV	756205	2989249	91.70%	15.830%
23	11.380	2986	2998	3026	rVB	666085	1169970	35.89%	6.196%
24	12.376	3295	3308	3332	rVB	524591	899012	27.58%	4.761%
25	13.087	3519	3529	3549	rVB6	47971	110235	3.38%	0.584%
26	13.318	3588	3601	3615	rBV	558094	969944	29.76%	5.137%
27	13.424	3625	3634	3646	rVB	144787	223650	6.86%	1.184%
28	13.489	3646	3654	3660	rBV3	28937	52413	1.61%	0.278%
29	13.646	3694	3703	3713	rBV	46443	66884	2.05%	0.354%
30	14.132	3836	3854	3860	rBV9	24175	57497	1.76%	0.304%
31	14.206	3871	3877	3889	rVB3	21842	38614	1.18%	0.204%
32	14.270	3890	3897	3903	rBV4	22437	32686	1.00%	0.173%
33	14.498	3959	3968	3977	rBV	192666	267681	8.21%	1.418%
34	14.563	3980	3988	3995	rVV7	22736	38737	1.19%	0.205%
35	14.614	3996	4004	4017	rVB2	66025	108030	3.31%	0.572%
36	15.010	4122	4127	4139	rVB3	57206	91230	2.80%	0.483%

LSC Area Percent Report

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Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Integration Parameters: RTEINT.P
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Title : SW846 8260

37	15.080	4140	4149	4162	rBV3	97557	183320	5.62%	0.971%
38	15.299	4208	4217	4231	rBV	177864	271050	8.32%	1.435%
39	15.730	4345	4351	4367	rVB5	21548	39314	1.21%	0.208%
40	15.993	4426	4433	4444	rVB2	22692	38291	1.17%	0.203%
41	16.193	4486	4495	4511	rVB	46386	85289	2.62%	0.452%

Sum of corrected areas: 18883063

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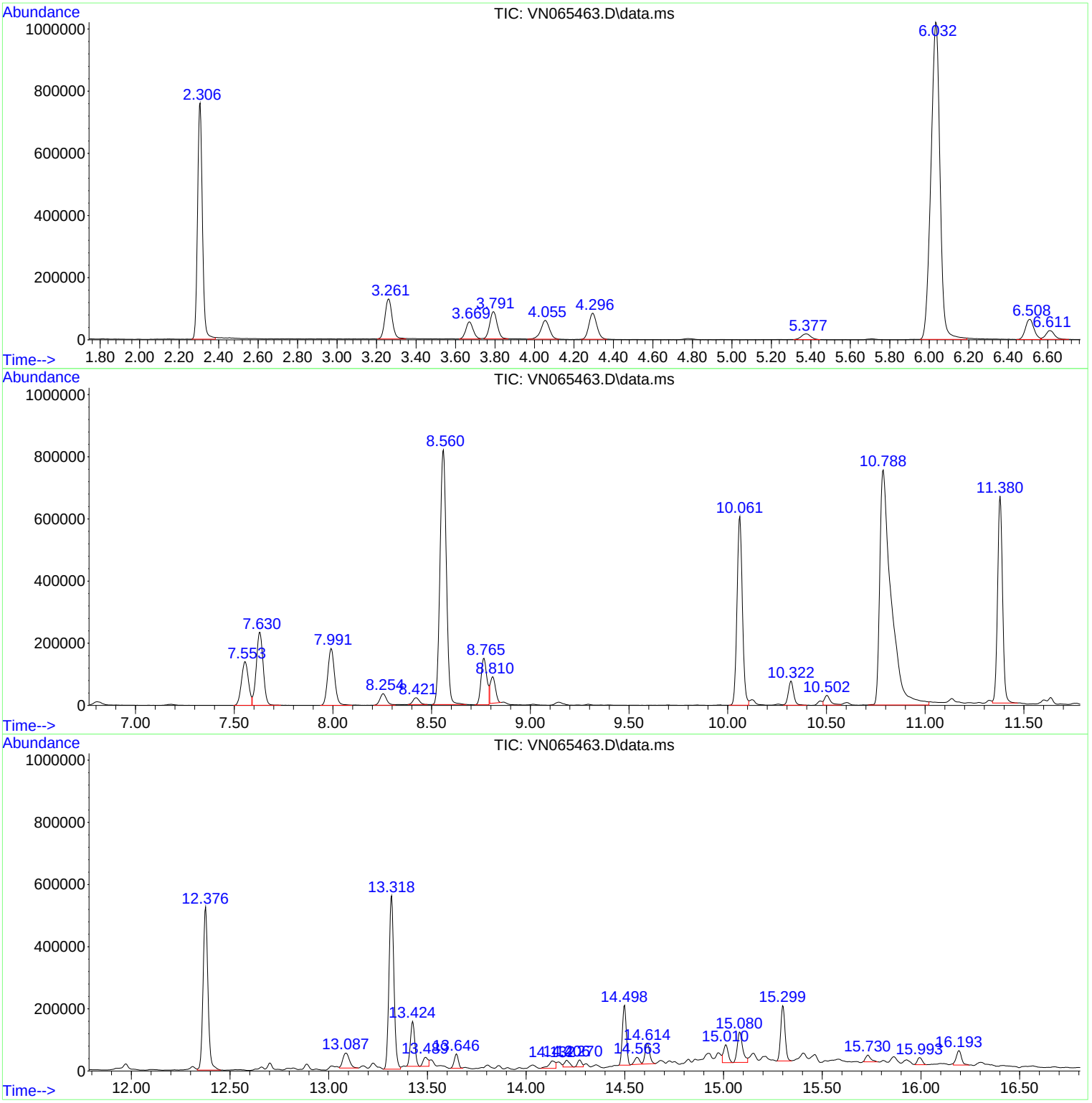
MSVOA_N
ClientSampleId :
41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
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Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

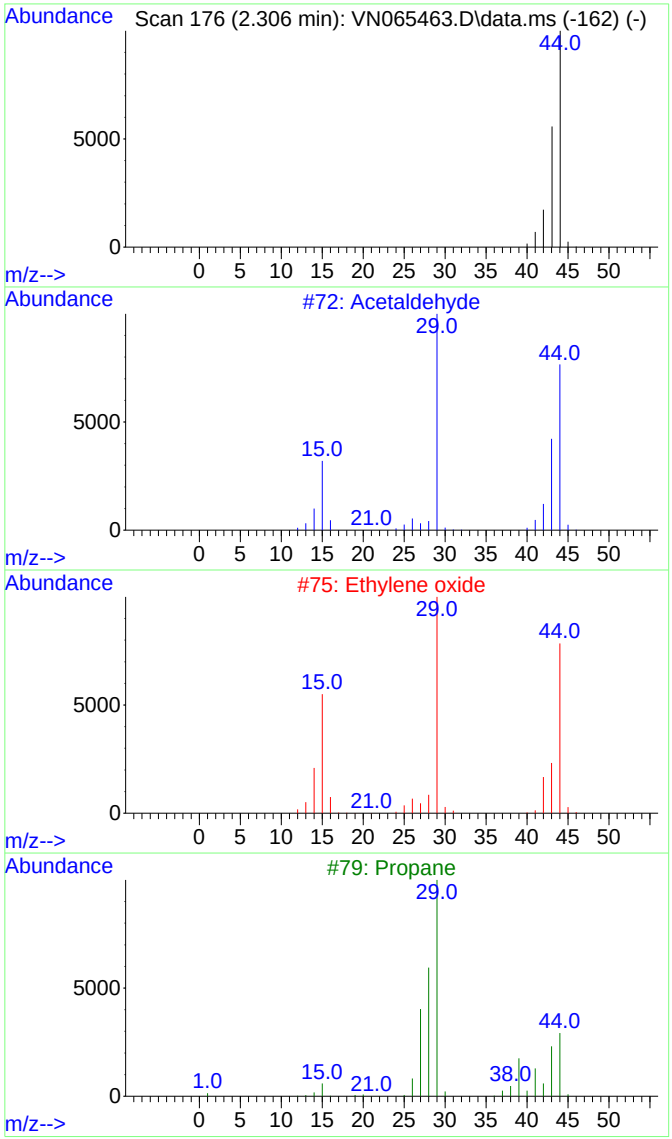
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

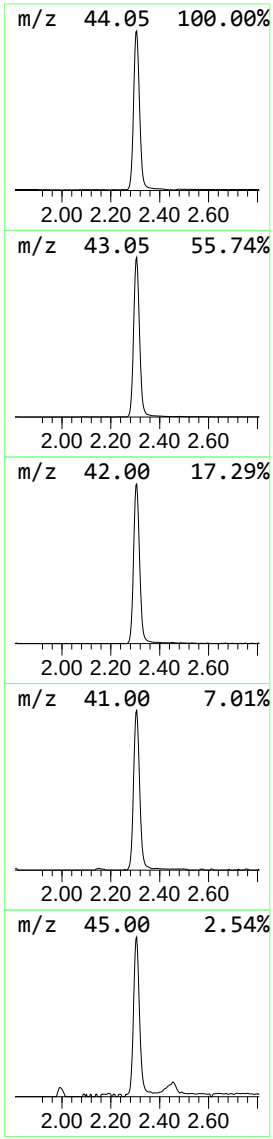
****

Peak Number 1 Acetaldehyde Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	114.47 ug/l	1288060	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyde	44	C2H4O	000075-07-0	74
2	Ethylene oxide	44	C2H4O	000075-21-8	5
3	Propane	44	C3H8	000074-98-6	4
4	Alanine	89	C3H7NO2	000056-41-7	4
5	1,2-Propanediamine	74	C3H10N2	000078-90-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

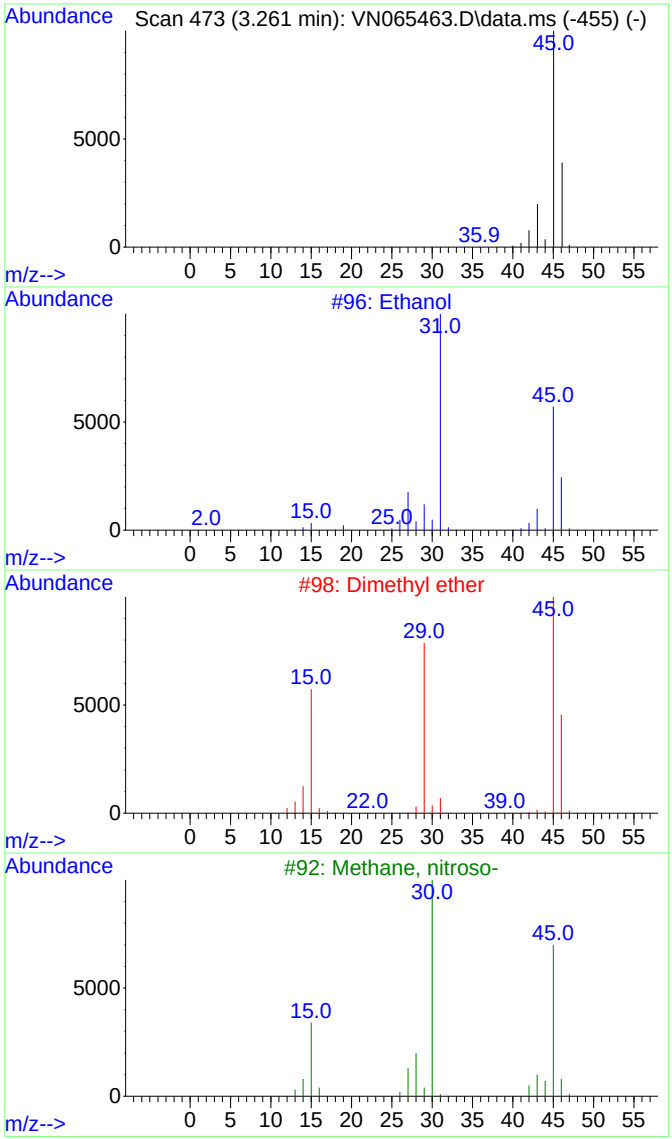
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

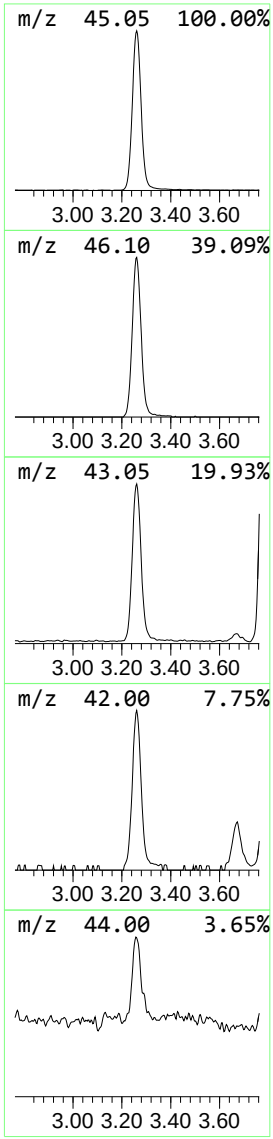
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Ethanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.261	28.95 ug/l	325758	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethanol	46	C2H6O	000064-17-5	74
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Methane, nitroso-	45	CH3NO	000865-40-7	4
4	Formic acid	46	CH2O2	000064-18-6	4
5	Oxalic acid	90	C2H2O4	000144-62-7	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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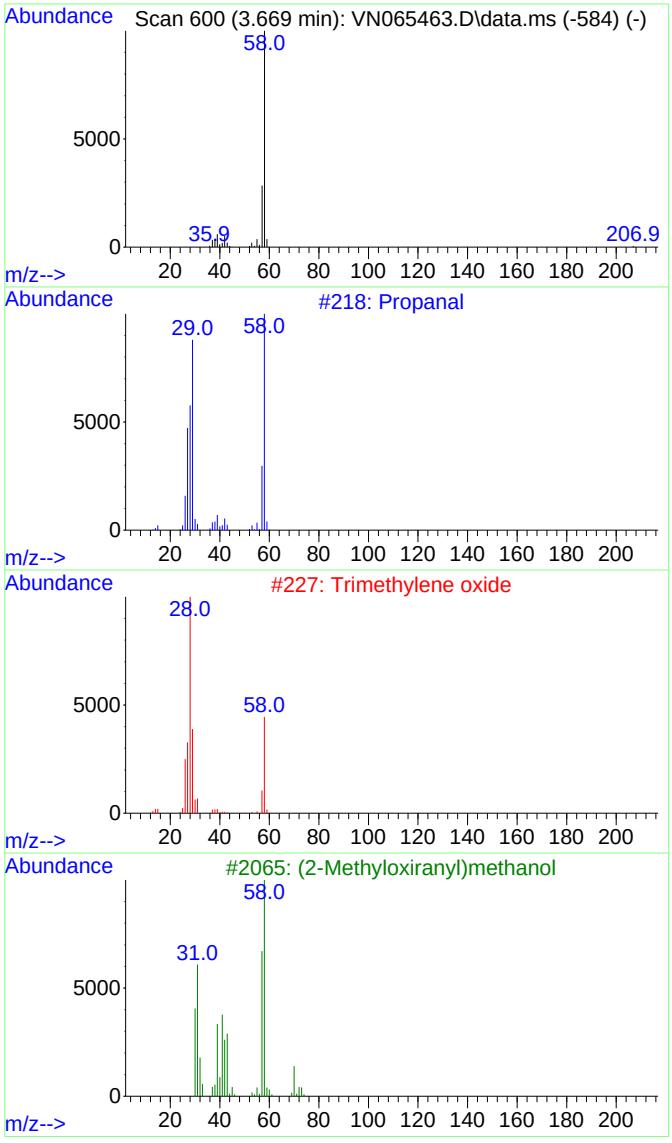
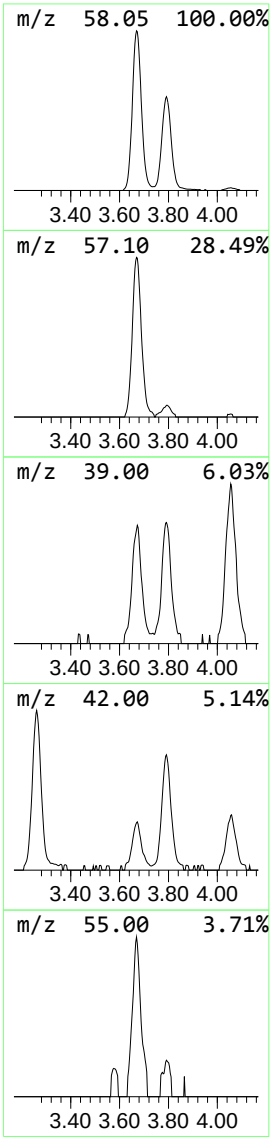
Peak Number 3 Propanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.669	12.58 ug/l	141522	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal	58	C3H6O	000123-38-6	72
2	Trimethylene oxide	58	C3H6O	000503-30-0	56
3	(2-Methyloxiranyl)methanol	88	C4H8O2	1000306-71-6	9
4	Hexanal, 2-methyl-	114	C7H14O	000925-54-2	9
5	Benzedrex	155	C10H21N	000101-40-6	9





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Data File : VN065463.D
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Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
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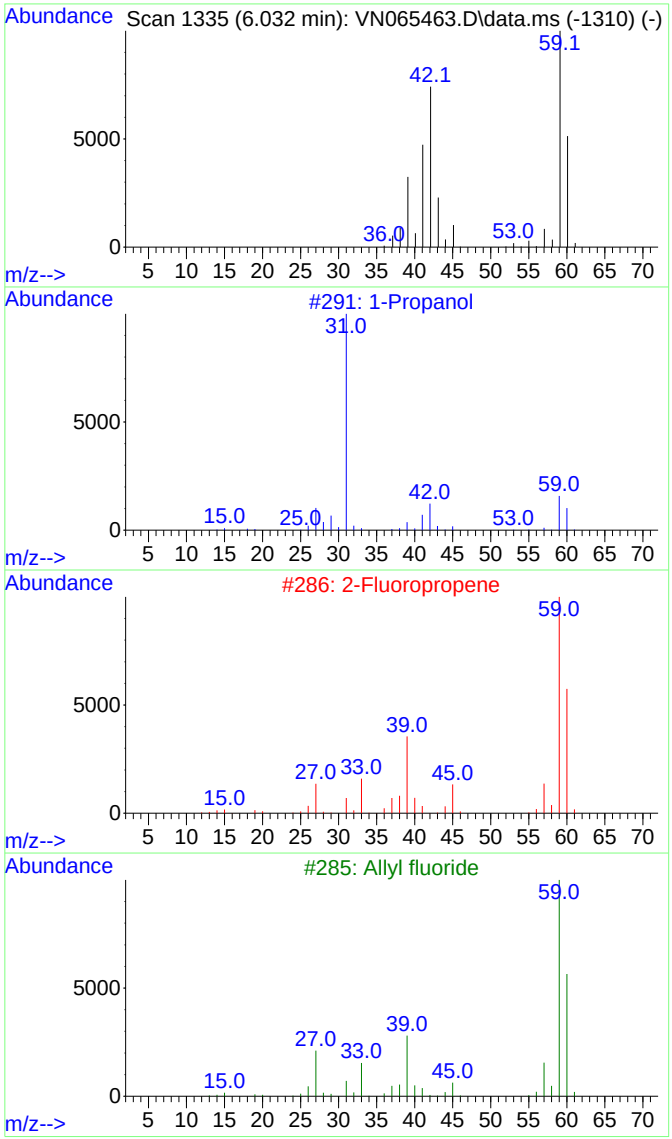
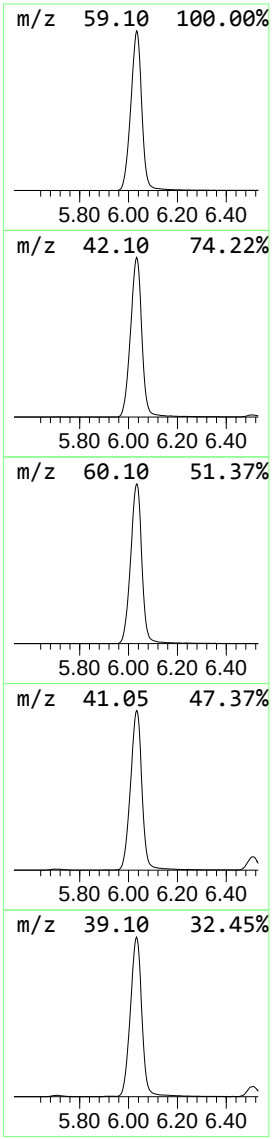
Peak Number 4 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.032	289.68 ug/l	3259670	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	78
2	2-Fluoropropene	60	C3H5F	001184-60-7	43
3	Allyl fluoride	60	C3H5F	000818-92-8	43
4	Acetaldoxime	59	C2H5NO	000107-29-9	7
5	Cyclopropane	42	C3H6	000075-19-4	7





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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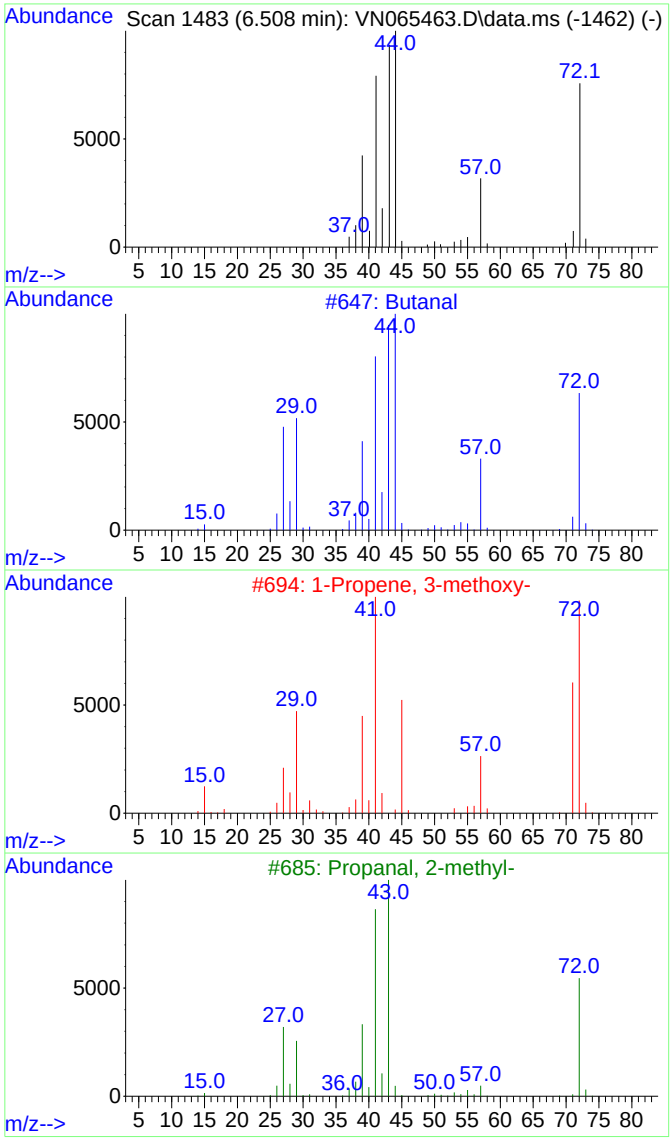
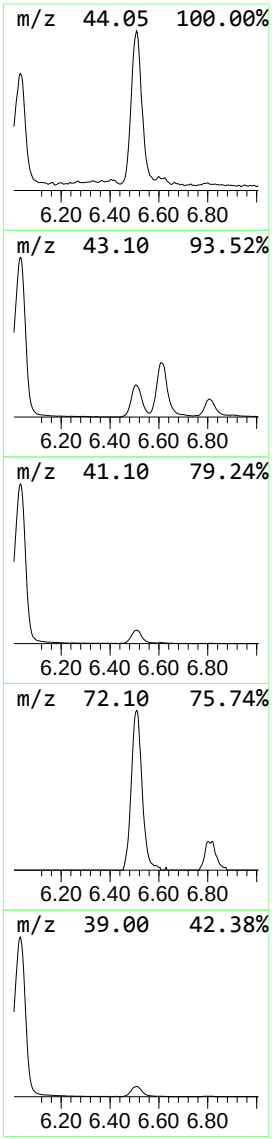
Peak Number 5 Butanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.508	17.39 ug/l	195730	Pentafluorobenzene	7.630

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	94
2	1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	47
3	Propanal, 2-methyl-	72	C4H8O	000078-84-2	46
4	Ethene, ethoxy-	72	C4H8O	000109-92-2	42
5	Isobutylene epoxide	72	C4H8O	000558-30-5	35





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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

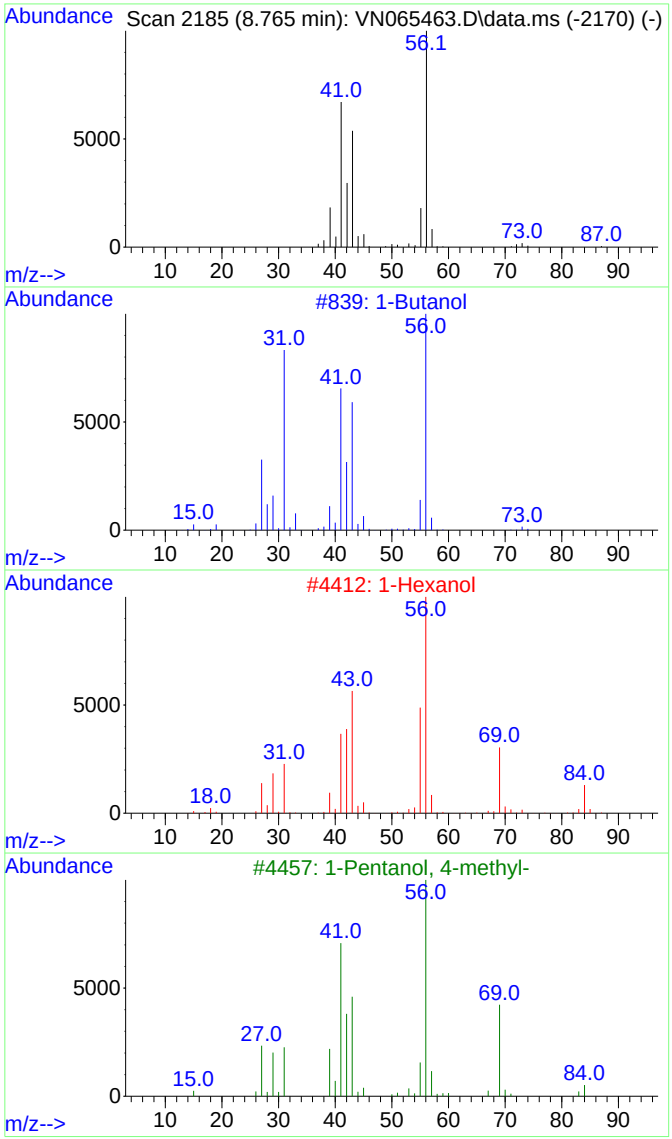
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

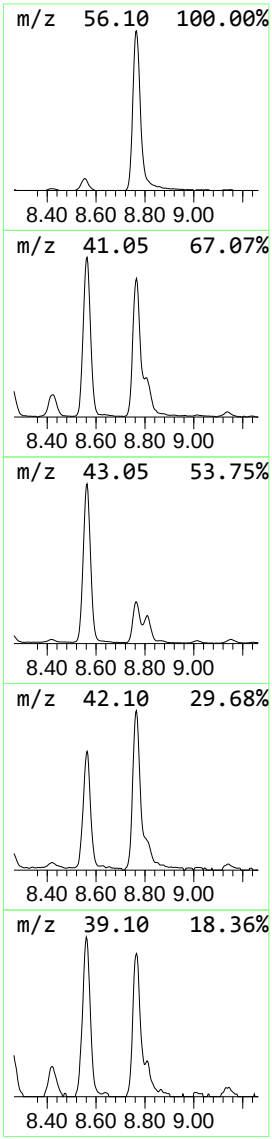
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 1-Butanol Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.765	8.56 ug/l	314795	1,4-Difluorobenzene	8.553

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Butanol	74	C4H10O	000071-36-3	90
2	1-Hexanol	102	C6H14O	000111-27-3	43
3	1-Pentanol, 4-methyl-	102	C6H14O	000626-89-1	40
4	2H-Pyran-2-one, tetrahydro-5,6-d...	128	C7H12O2	024405-16-1	38
5	Formic acid, butyl ester	102	C5H10O2	000592-84-7	9





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Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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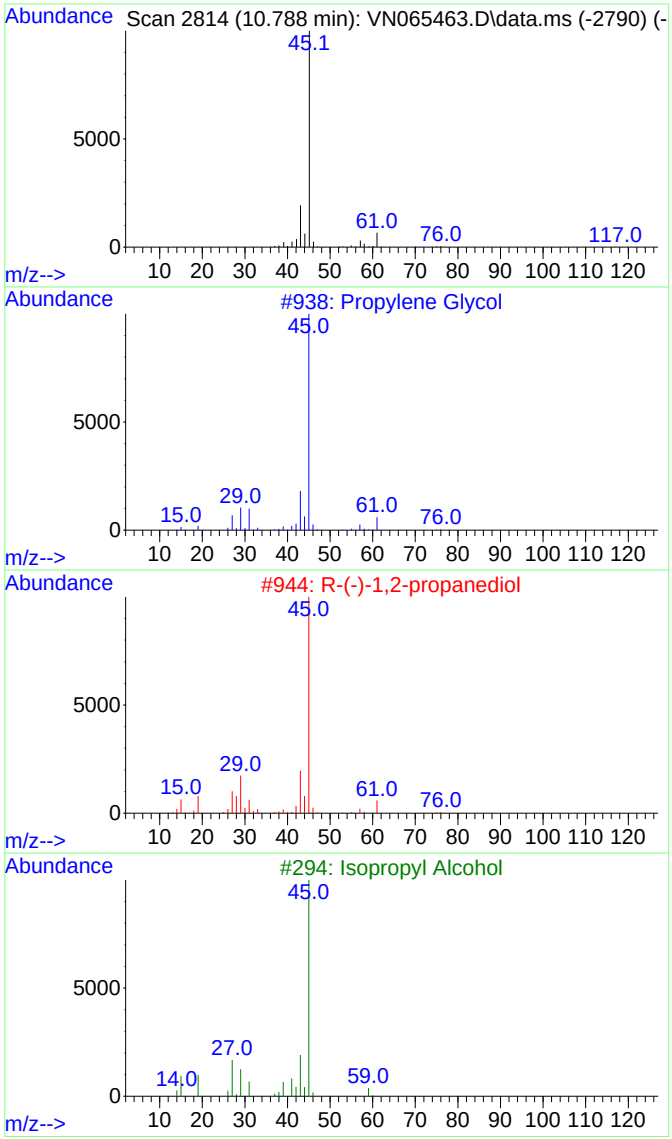
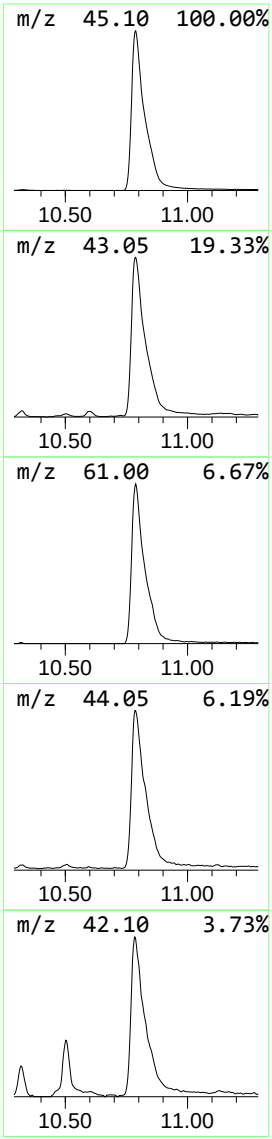
Peak Number 7 Propylene Glycol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.788	127.75 ug/l	2989250	Chlorobenzene-d5	11.380

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	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	2-Butanol	74	C4H10O	000078-92-2	9





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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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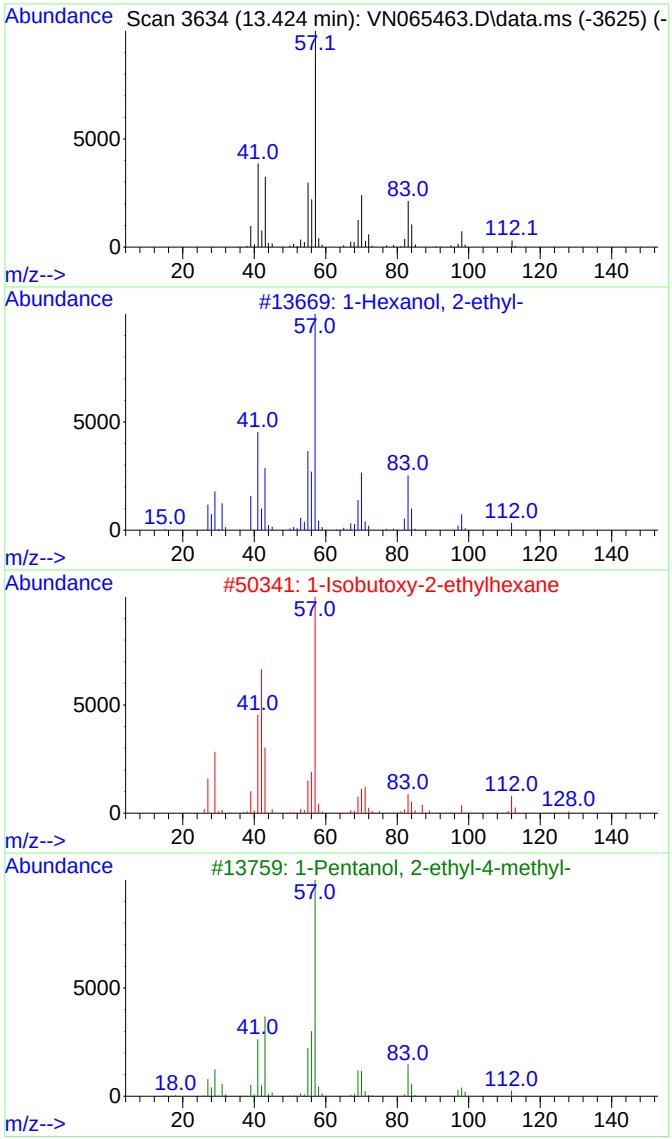
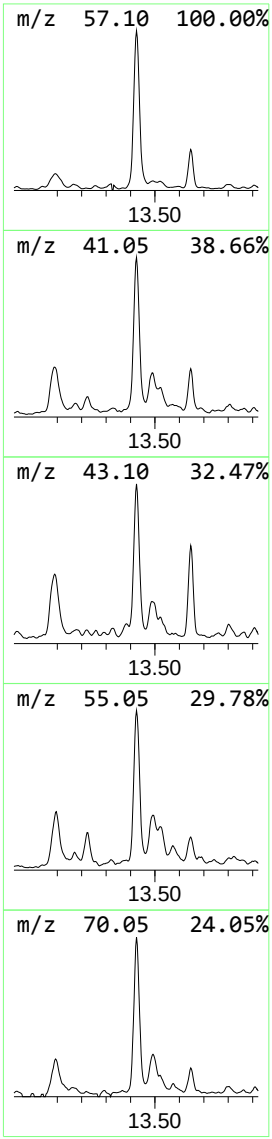
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.424	11.53 ug/l	223650	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	59
3	1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	56
4	2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
5	Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45





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Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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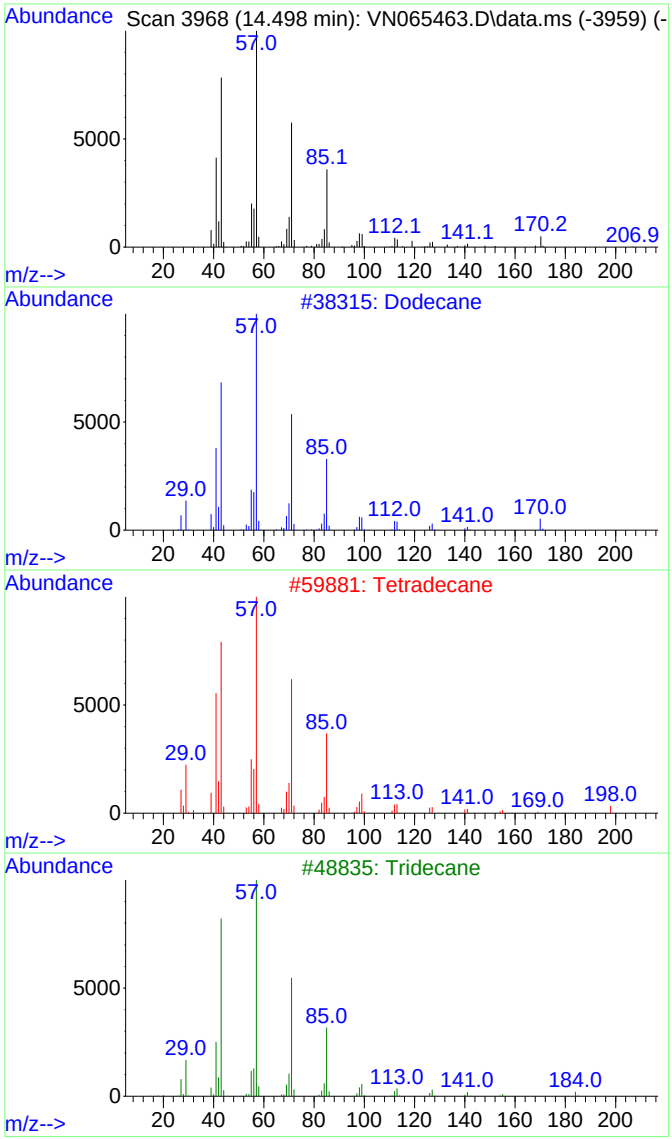
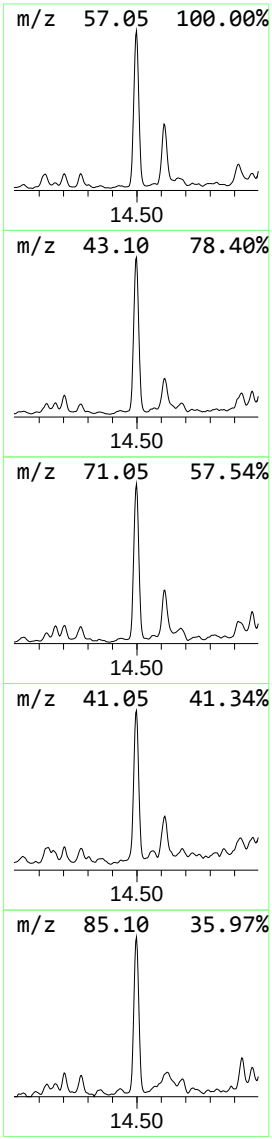
Peak Number 9 Dodecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.498	13.80 ug/l	267681	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecane	170	C12H26	000112-40-3	96
2	Tetradecane	198	C14H30	000629-59-4	91
3	Tridecane	184	C13H28	000629-50-5	90
4	Undecane	156	C11H24	001120-21-4	90
5	Hexadecane	226	C16H34	000544-76-3	87





Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

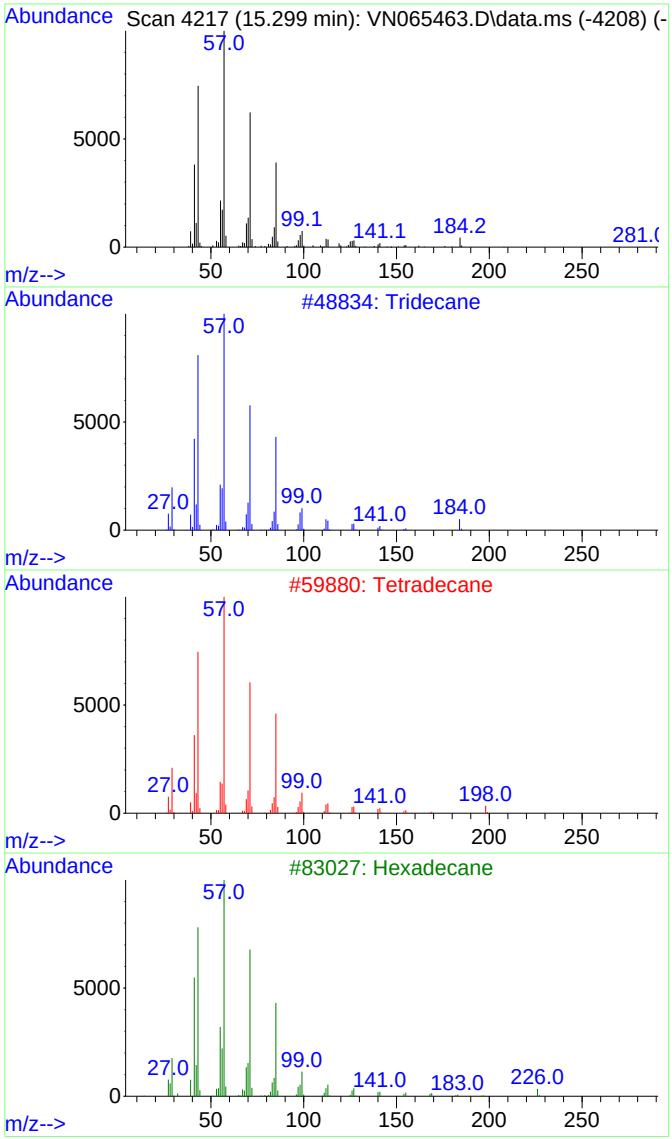
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

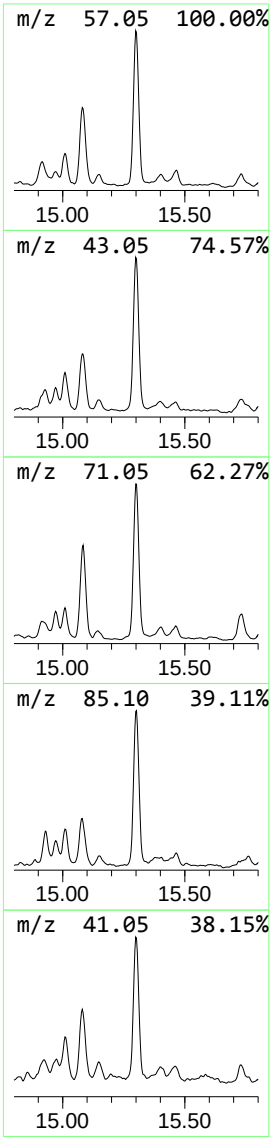
****

Peak Number 10 Tridecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.299	13.97 ug/l	271050	1,4-Dichlorobenzene-d4	13.318

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecane	184	C13H28	000629-50-5	96
2	Tetradecane	198	C14H30	000629-59-4	87
3	Hexadecane	226	C16H34	000544-76-3	87
4	Dodecane	170	C12H26	000112-40-3	86
5	Decane, 2,3,6-trimethyl-	184	C13H28	062238-12-4	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN011121\
Data File : VN065463.D
Acq On : 11 Jan 2021 13:12
Operator : JC/MD
Sample : M1022-07
Misc : 5.00mL/MSVOA_N/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : 41038

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122220W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	2.306	114.5	ug/l	1288060	1	7.630	562639	50.0
Ethanol	3.261	28.9	ug/l	325758	1	7.630	562639	50.0
Propanal	3.669	12.6	ug/l	141522	1	7.630	562639	50.0
1-Propanol	6.032	289.7	ug/l	3259670	1	7.630	562639	50.0
Butanal	6.508	17.4	ug/l	195730	1	7.630	562639	50.0
1-Butanol	8.765	8.6	ug/l	314795	2	8.553	1838980	50.0
Propylene Glycol	10.788	127.8	ug/l	2989250	3	11.380	1169970	50.0
1-Hexanol, 2-et...	13.424	11.5	ug/l	223650	4	13.318	969944	50.0
Dodecane	14.498	13.8	ug/l	267681	4	13.318	969944	50.0
Tridecane	15.299	14.0	ug/l	271050	4	13.318	969944	50.0