LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN083024\
Data File : VN083597.D
Acq On : 31 Aug 2024 06:09
Operator : JC\MD
Sample : P3769-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : MW-09-6.5-082724

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\82N083024W.M
Title : SW846 8260

Signal : TIC: VN083597.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.077	16	21	26	rVV	59845	86119	8.27%	1.270%
2	2.124	26	29	37	rVB2	21626	34103	3.28%	0.503%
3	2.230	42	47	52	rBV	42943	67278	6.46%	0.992%
4	2.295	52	58	59	rBV3	46186	69143	6.64%	1.020%
5	2.324	59	63	70	rVB	101834	162655	15.62%	2.399%
6	2.518	91	96	104	rVB2	17850	30316	2.91%	0.447%
7	2.606	105	111	117	rBV	32588	58317	5.60%	0.860%
8	2.830	139	149	150	rBV4	10811	26675	2.56%	0.393%
9	3.071	182	190	202	rVB2	47688	114441	10.99%	1.688%
10	4.053	344	357	369	rBV2	48343	138311	13.28%	2.040%
11	4.353	399	408	415	rBV2	34089	103066	9.90%	1.520%
12	4.436	415	422	433	rVB	59851	176130	16.91%	2.598%
13	7.489	931	941	950	rBV2	37267	96867	9.30%	1.429%
14	8.165	1047	1056	1060	rBV	134818	309656	29.74%	4.567%
15	8.224	1060	1066	1079	rVB	215778	478422	45.95%	7.056%
16	8.577	1117	1126	1135	rBV	143078	313251	30.08%	4.620%
17	9.100	1206	1215	1226	rBV	360656	732037	70.30%	10.797%
18	10.565	1454	1464	1472	rBV	512703	929075	89.22%	13.703%
19	11.865	1677	1685	1695	rBV	585887	1041286	100.00%	15.358%
20	12.847	1845	1852	1860	rVB	461200	772635	74.20%	11.396%
21	13.788	2005	2012	2021	rBV	625348	1040357	99.91%	15.344%

Sum of corrected areas: 6780140

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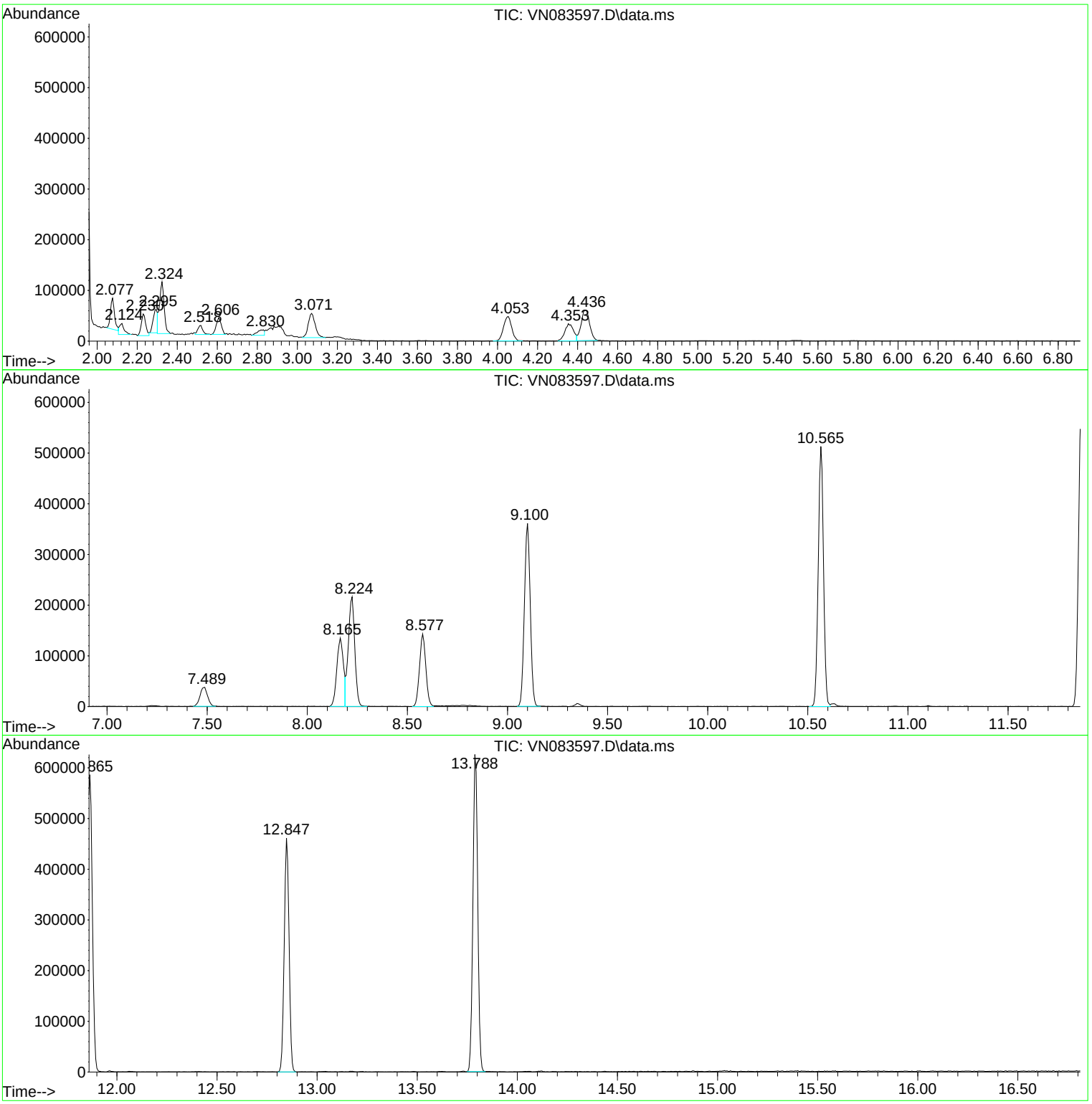
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-6.5-082724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

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



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Data File : VN083597.D
Acq On : 31 Aug 2024 06:09
Operator : JC\MD
Sample : P3769-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

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ClientSampleId :
MW-09-6.5-082724

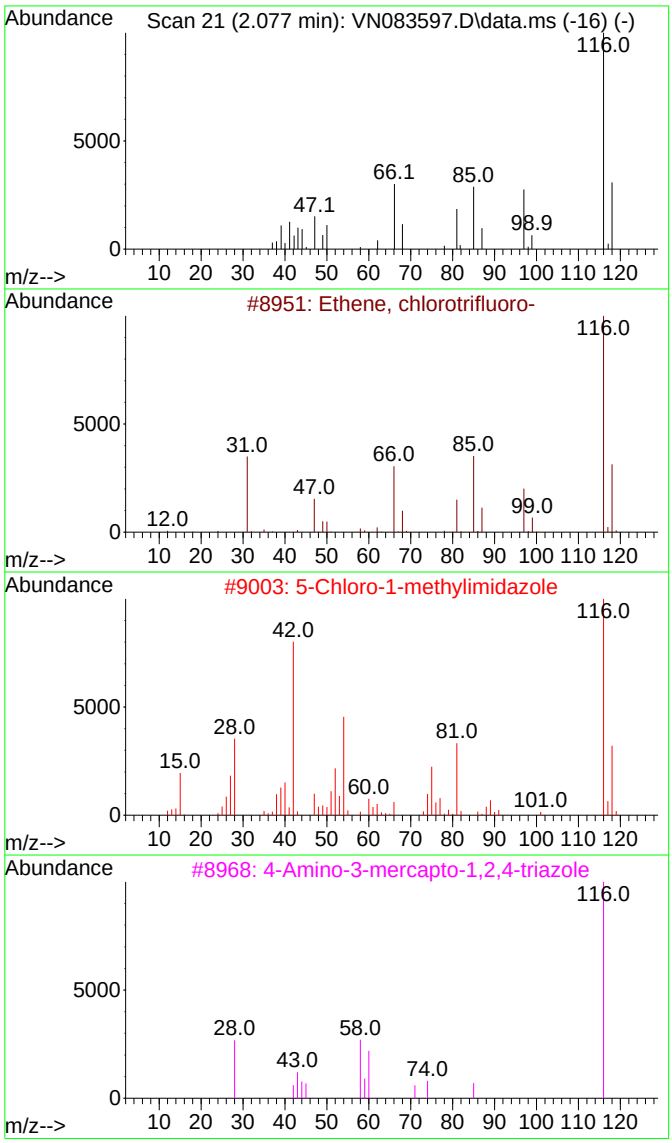
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

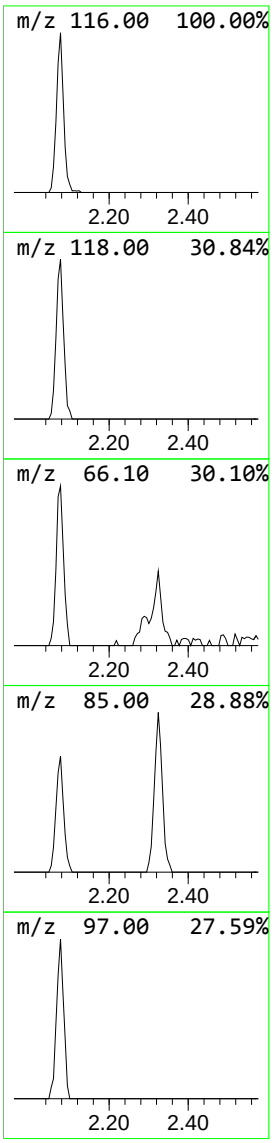
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Ethene, chlorotrifluoro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.077	9.00 ug/l	86119	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethene, chlorotrifluoro-	116	C2ClF3	000079-38-9	94
2	5-Chloro-1-methylimidazole	116	C4H5ClN2	000872-49-1	9
3	4-Amino-3-mercapto-1,2,4-triazole	116	C2H4N4S	004343-75-3	7
4	1-Propene, 1-(ethylthio)-2-methyl-	116	C6H12S	027482-14-0	5
5	Butanethiol, 1,3-diimino-	116	C4H8N2S	032081-55-3	4





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ALS Vial : 42 Sample Multiplier: 1

Instrument :
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ClientSampleId :
MW-09-6.5-082724

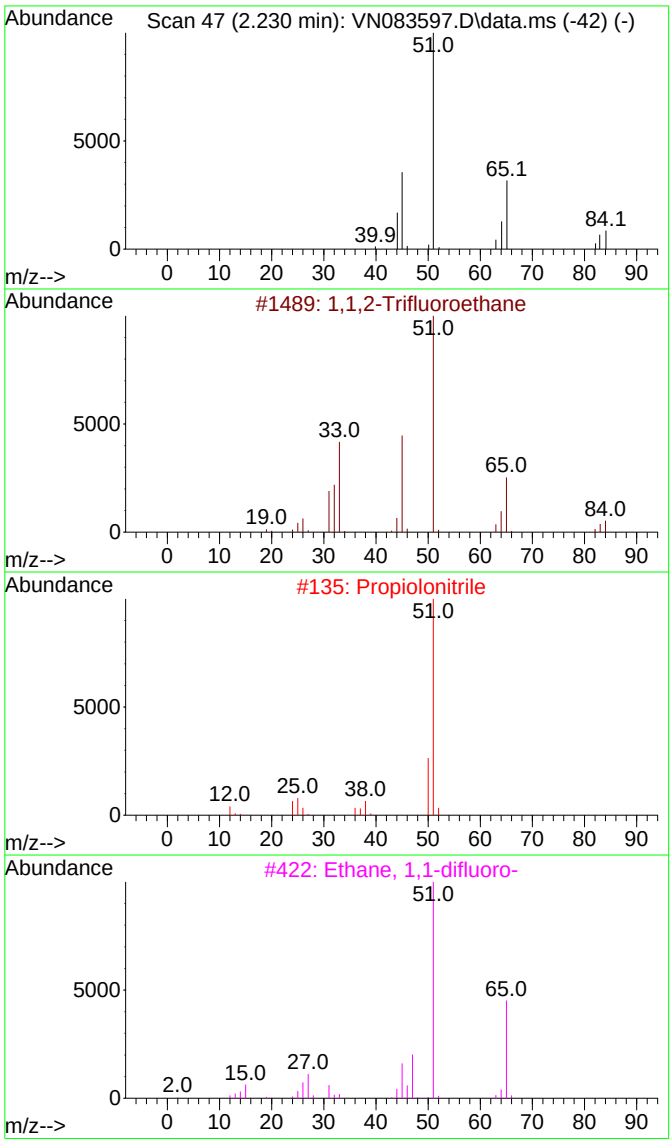
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

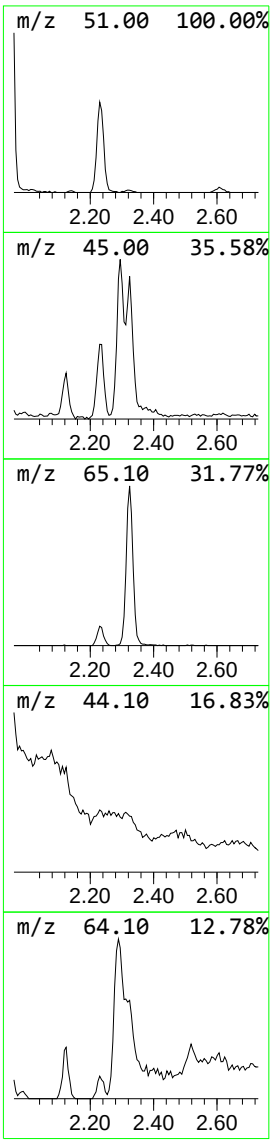
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,1,2-Trifluoroethane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.230	7.03 ug/l	67278	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1,2-Trifluoroethane	84	C2H3F3	000430-66-0	90
2	Propiolonitrile	51	C3HN	001070-71-9	3
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	2
4	Difluoromethyl trifluoromethanes...	200	C2HF5O3S	001885-46-7	1
5	Norflurane	102	C2H2F4	000811-97-2	1





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Data File : VN083597.D
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Operator : JC\MD
Sample : P3769-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-6.5-082724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

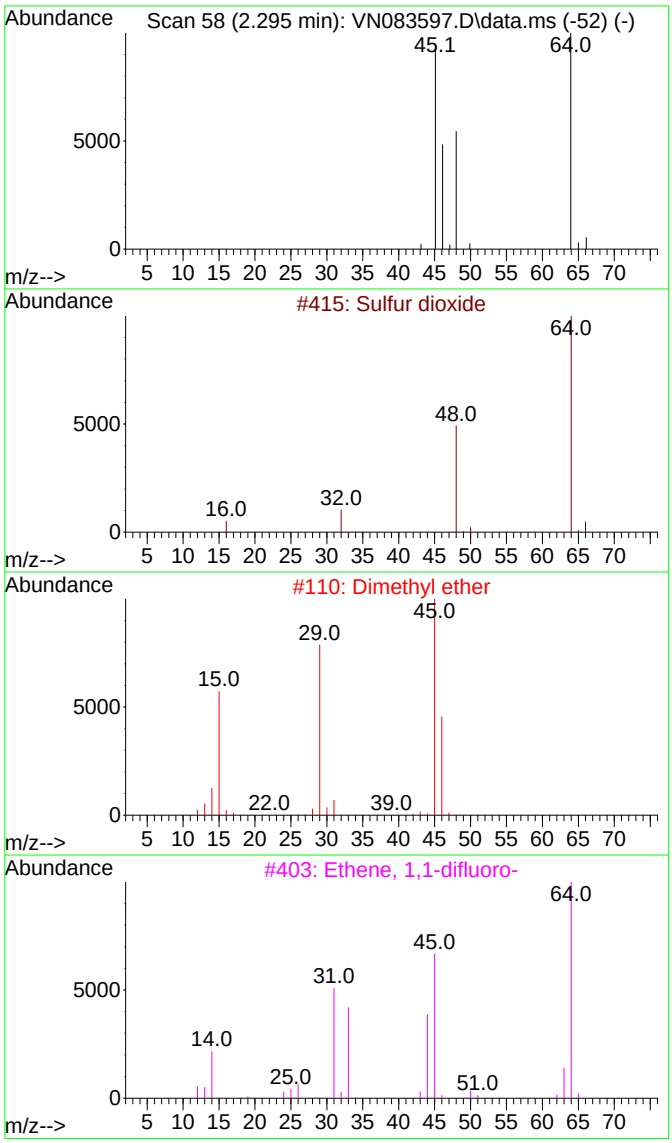
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

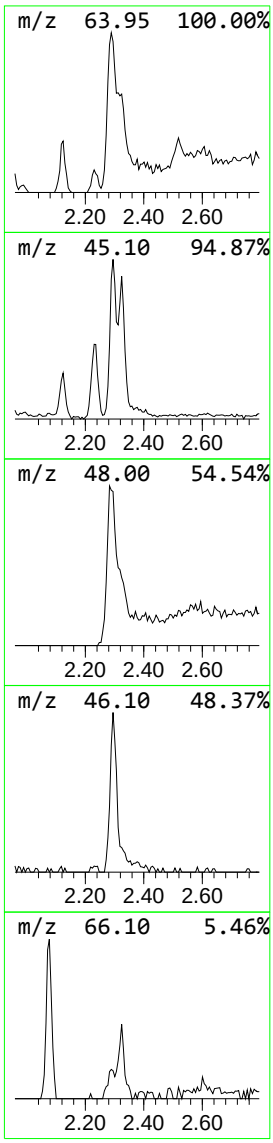
****

Peak Number 3 unknown2.295 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.295	7.23 ug/l	69143	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	45
2	Dimethyl ether	46	C2H6O	000115-10-6	9
3	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9





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Data File : VN083597.D
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Operator : JC\MD
Sample : P3769-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-6.5-082724

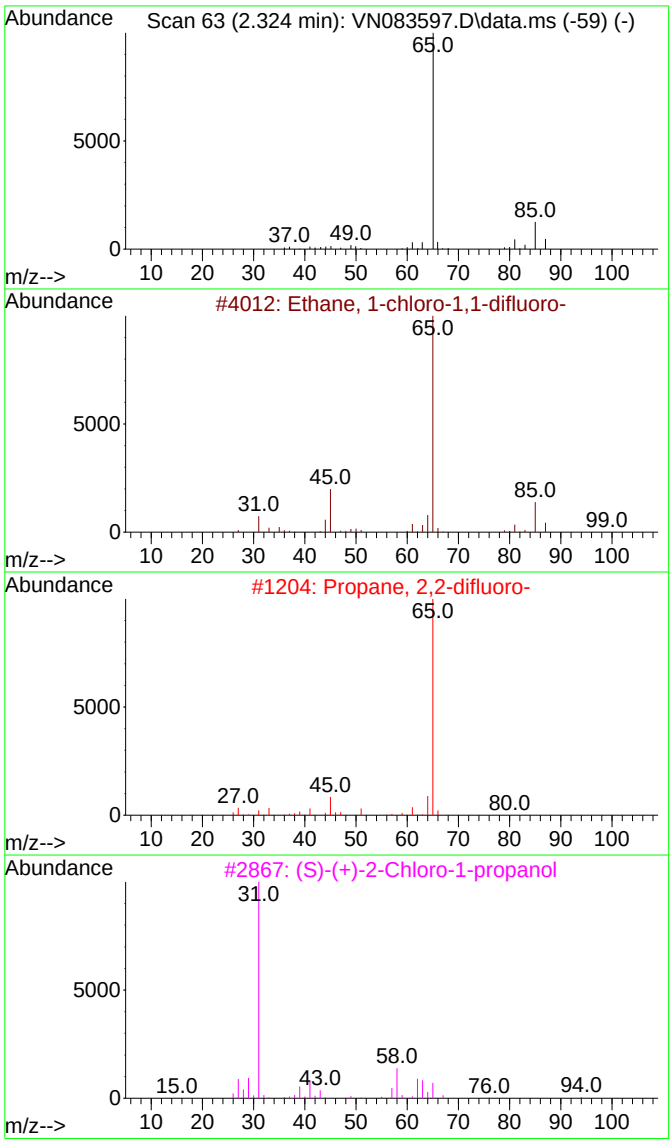
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

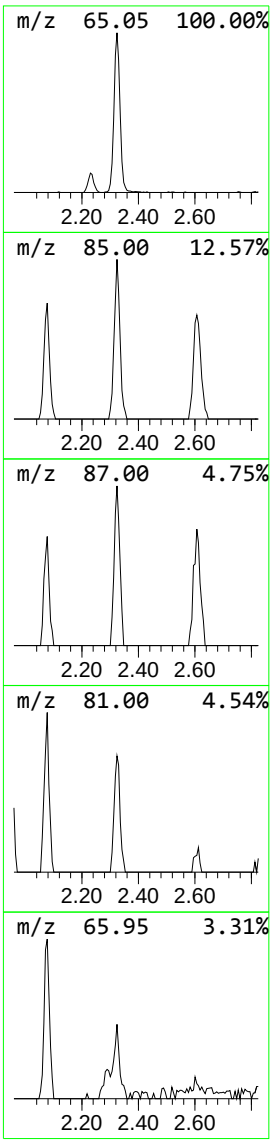
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Ethane, 1-chloro-1,1-difluoro- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.324	17.00 ug/l	162655	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-chloro-1,1-difluoro-	100	C2H3ClF2	000075-68-3	74
2	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	9
3	(S)-(+)-2-Chloro-1-propanol	94	C3H7ClO	019210-21-0	1
4	1-Propanol, 2-chloro-	94	C3H7ClO	000078-89-7	1
5	Ethyl fluoroformate	92	C3H5FO2	000461-64-3	1





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Data File : VN083597.D
Acq On : 31 Aug 2024 06:09
Operator : JC\MD
Sample : P3769-01
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-6.5-082724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

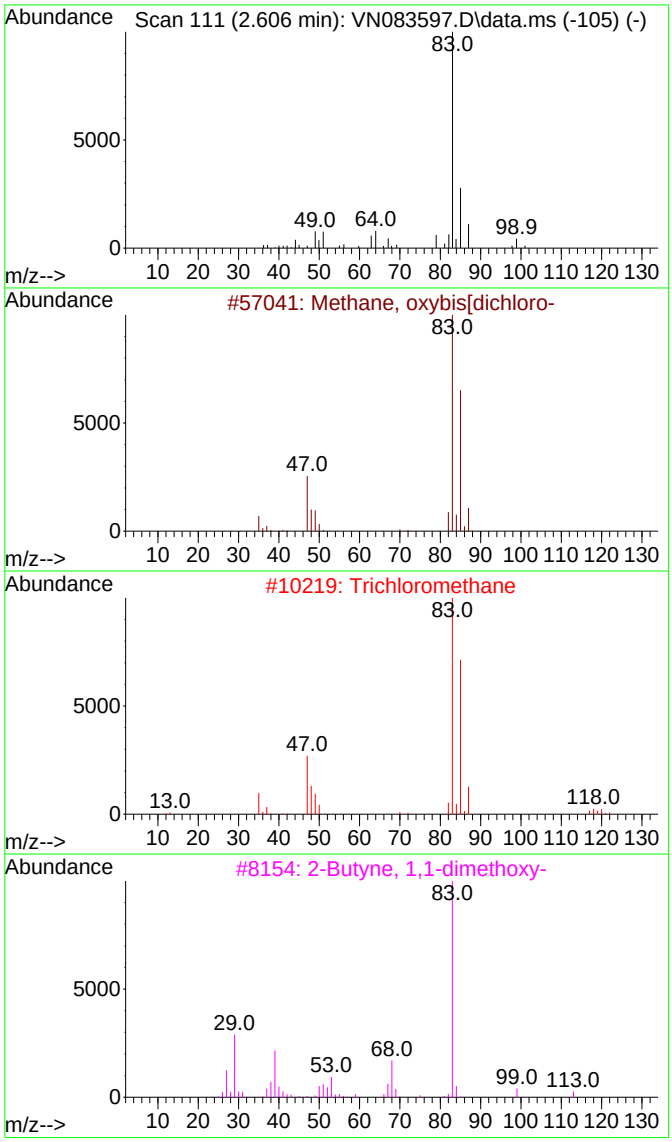
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

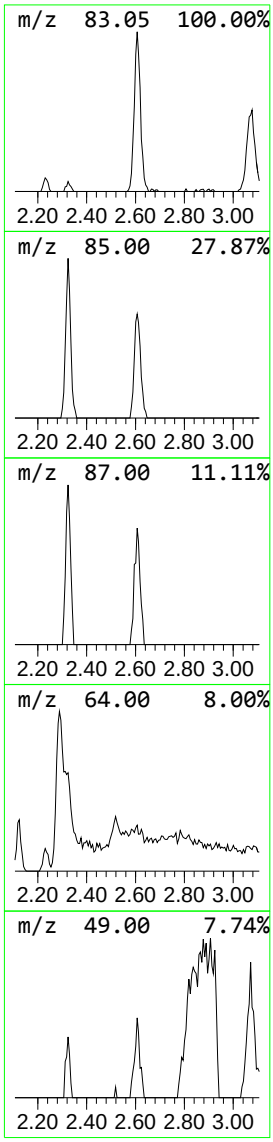
****

Peak Number 5 unknown2.606 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.606	6.09 ug/l	58317	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methane, oxybis[dichloro-	182	C2H2Cl4O	020524-86-1	36
2	Trichloromethane	118	CHCl3	000067-66-3	36
3	2-Butyne, 1,1-dimethoxy-	114	C6H10O2	022022-34-0	33
4	3-Aminopyrazole	83	C3H5N3	001820-80-0	9
5	Hexanal 2E-hexenyl 3Z-hexenyl ac...	282	C18H34O2	1000431-43-4	9





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Operator : JC\MD
Sample : P3769-01
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ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-09-6.5-082724

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N083024W.M
Quant Title : SW846 8260

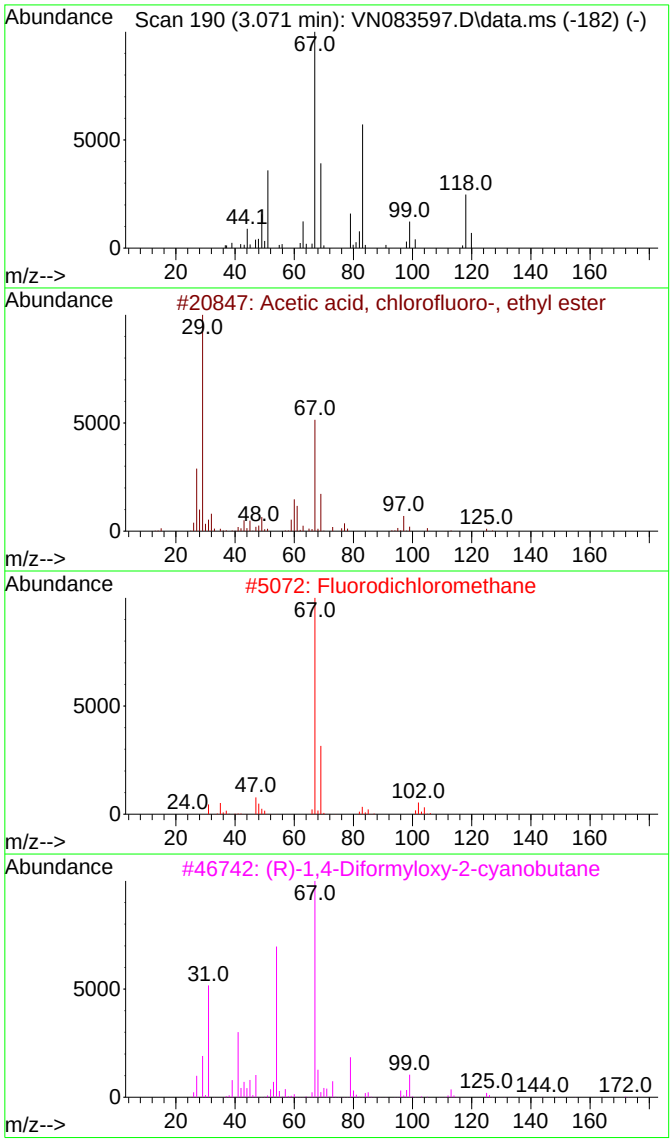
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

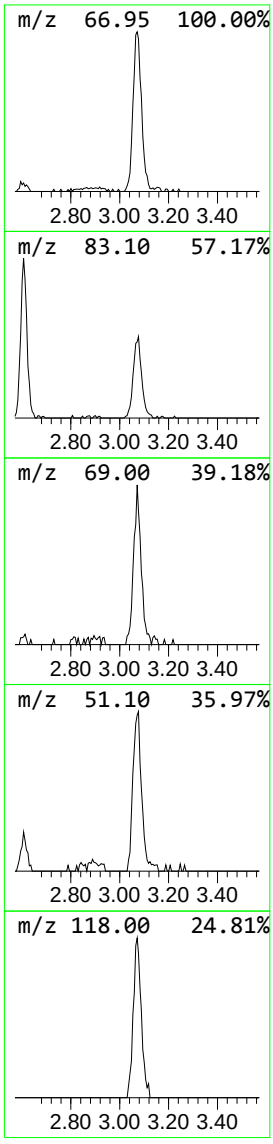
****

Peak Number 6 unknown3.071 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.071	11.96 ug/l	114441	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chlorofluoro-, ethy...	140	C4H6ClFO2	000401-56-9	23
2	Fluorodichloromethane	102	CHCl2F	000075-43-4	9
3	(R)-1,4-Diformyloxy-2-cyanobutane	171	C7H9NO4	1000159-47-4	9
4	dl-Noformicin sulfate	197	C8H15N5O	1000131-37-1	9
5	Ethane, 2-chloro-1,1,1,2-tetrafl...	136	C2HClF4	002837-89-0	9





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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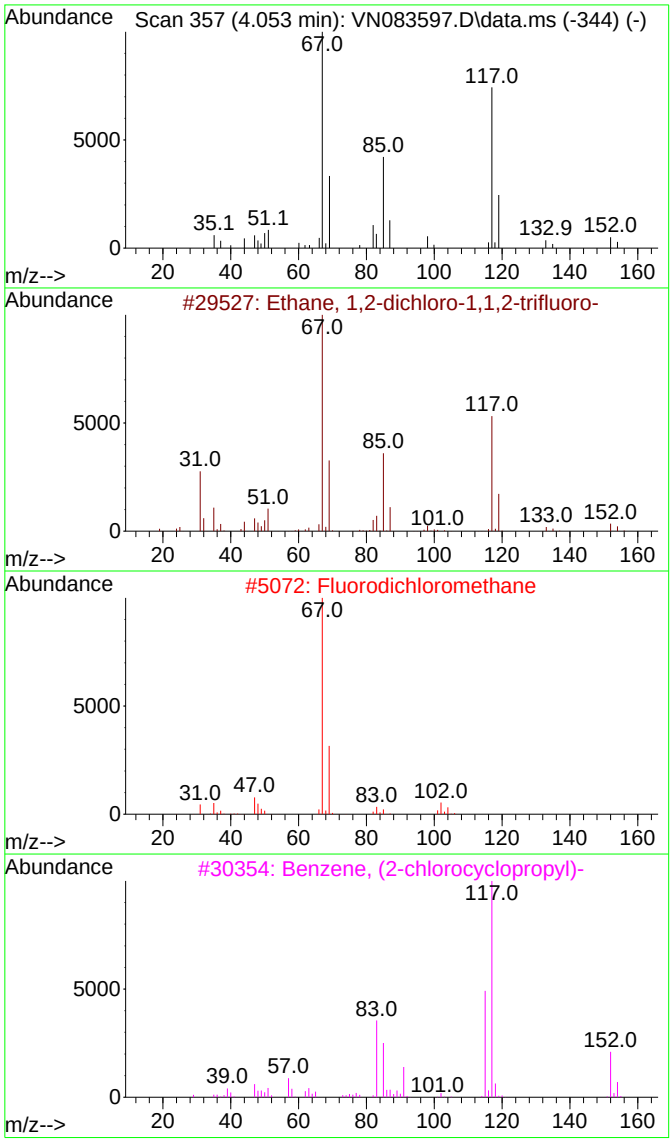
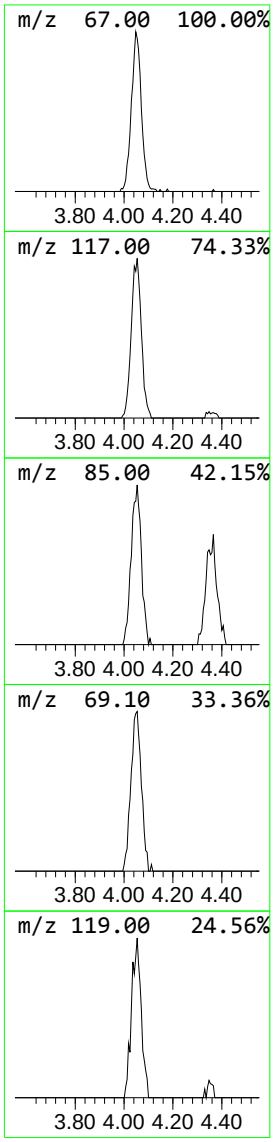
****
Peak Number 7 Ethane, 1,2-dichloro-1,1,2-... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.053	14.45 ug/l	138311	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,2-dichloro-1,1,2-trifl...	152	C2HCl2F3	000354-23-4	91
2	Fluorodichloromethane	102	CHCl2F	000075-43-4	12
3	Benzene, (2-chlorocyclopropyl)-	152	C9H9Cl	1000327-31-4	12
4	Cyclopropane, 1,2-dimethyl-3-met...	82	C6H10	062338-02-7	10
5	2,3-Butanediol, 2TMS derivative	234	C10H26O2Si2	053274-85-4	10





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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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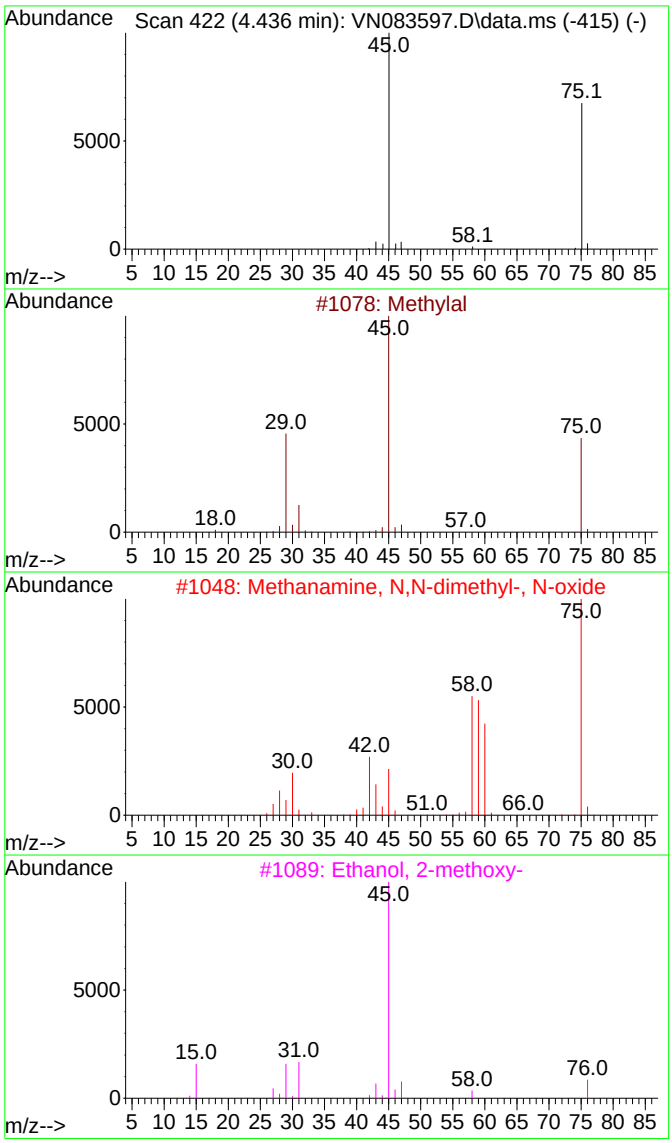
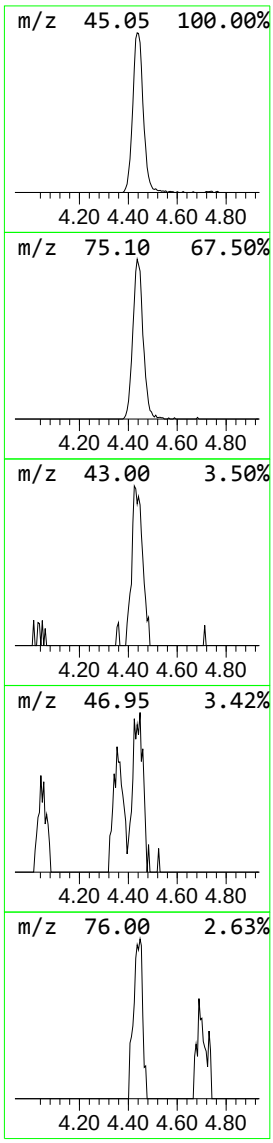
****
Peak Number 8 Methylal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.436	18.41 ug/l	176130	Pentafluorobenzene	8.224

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylal	76	C3H8O2	000109-87-5	83
2	Methanamine, N,N-dimethyl-, N-oxide	75	C3H9NO	001184-78-7	9
3	Ethanol, 2-methoxy-	76	C3H8O2	000109-86-4	9
4	Glycine	75	C2H5NO2	000056-40-6	4
5	Formamide	45	CH3NO	000075-12-7	4





Tentatively Identified Compound (LSC) summary

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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
Ethene, chlorot...	2.077	9.0	ug/l	86119	1	8.224	478422	50.0
1,1,2-Trifluoro...	2.230	7.0	ug/l	67278	1	8.224	478422	50.0
unknown2.295	2.295	7.2	ug/l	69143	1	8.224	478422	50.0
Ethane, 1-chlor...	2.324	17.0	ug/l	162655	1	8.224	478422	50.0
unknown2.606	2.606	6.1	ug/l	58317	1	8.224	478422	50.0
unknown3.071	3.071	12.0	ug/l	114441	1	8.224	478422	50.0
Ethane, 1,2-dic...	4.053	14.4	ug/l	138311	1	8.224	478422	50.0
Methylal	4.436	18.4	ug/l	176130	1	8.224	478422	50.0