LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN101123\
Data File : VN079521.D
Acq On : 11 Oct 2023 16:48
Operator : JC\MD
Sample : 04823-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

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\82N100523W.M
Title : SW846 8260

Signal : TIC: VN079521.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.659	109	120	132	rBV	5810004	10090209	16.62%	5.640%
2	4.242	387	389	390	rBV	40166418	28926700	47.66%	16.168%
3	4.430	415	421	461	rVB	3094935	10972124	18.08%	6.132%
4	4.724	463	471	486	rVB	234240	755633	1.24%	0.422%
5	5.589	599	618	639	rBV2	432060	1491773	2.46%	0.834%
6	6.800	788	824	841	rBV	14062109	60697646	100.00%	33.925%
7	8.171	1047	1057	1061	rBV	428757	983932	1.62%	0.550%
8	8.230	1061	1067	1081	rVB	675781	1543400	2.54%	0.863%
9	8.606	1115	1131	1138	rBV3	1233763	3593059	5.92%	2.008%
10	8.671	1138	1142	1151	rVB2	317254	661448	1.09%	0.370%
11	8.983	1184	1195	1201	rBV	409012	918622	1.51%	0.513%
12	9.106	1208	1216	1234	rVB	1045153	2138879	3.52%	1.195%
13	10.571	1457	1465	1470	rBV	1654598	3072949	5.06%	1.718%
14	10.635	1470	1476	1483	rVV	2798744	5049454	8.32%	2.822%
15	10.724	1483	1491	1504	rVB	8542672	15199882	25.04%	8.495%
16	11.829	1672	1679	1683	rBV2	5094515	9423097	15.52%	5.267%
17	11.871	1683	1686	1690	rVV	1579139	2650609	4.37%	1.481%
18	11.912	1690	1693	1698	rVV	737276	1223490	2.02%	0.684%
19	11.971	1698	1703	1712	rVV	487615	897430	1.48%	0.502%
20	12.071	1712	1720	1729	rVB	1496404	2801278	4.62%	1.566%
21	12.400	1771	1776	1794	rVB3	833140	1698642	2.80%	0.949%
22	12.800	1834	1844	1848	rBV	844682	1381534	2.28%	0.772%
23	12.853	1848	1853	1865	rVB	1237276	2129703	3.51%	1.190%
24	13.482	1953	1960	1966	rBV2	390786	788318	1.30%	0.441%
25	13.635	1980	1986	1991	rBV	409514	635391	1.05%	0.355%
26	13.794	2006	2013	2023	rBV2	1378870	2563437	4.22%	1.433%
27	15.647	2320	2328	2339	rVB	3426591	6629373	10.92%	3.705%

Sum of corrected areas: 178918012

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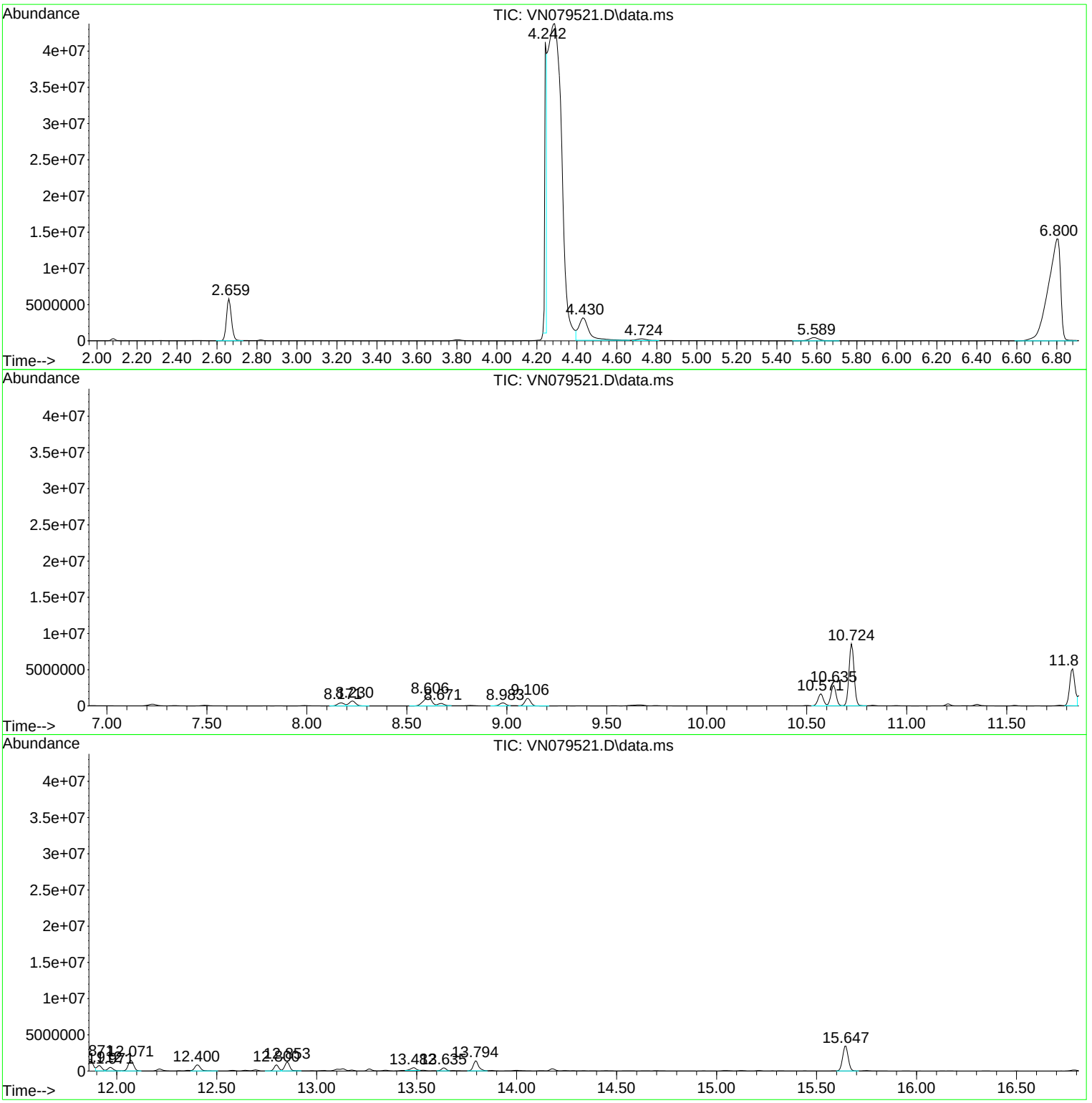
ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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



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Instrument :
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ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

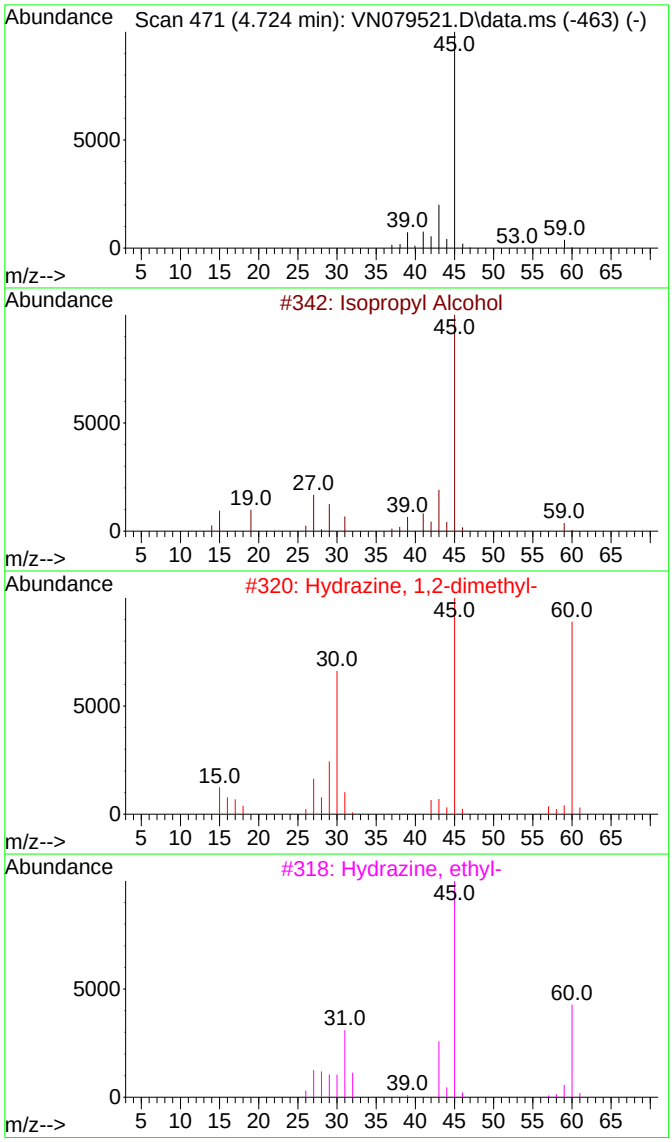
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

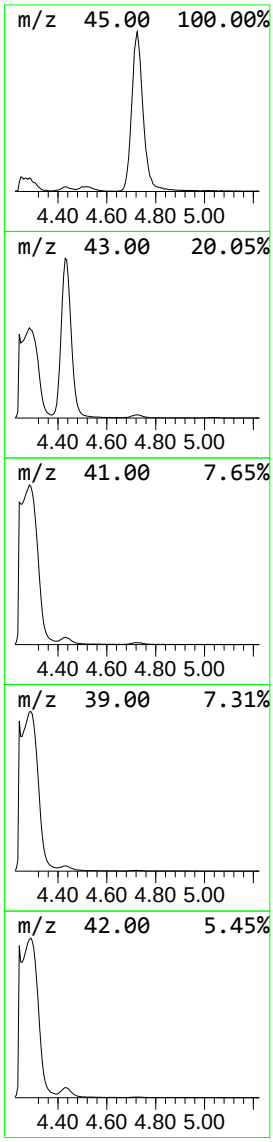
****

Peak Number 3 Isopropyl Alcohol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.724	24.48 ug/l	755633	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	83
2	Hydrazine, 1,2-dimethyl-	60	C2H8N2	000540-73-8	9
3	Hydrazine, ethyl-	60	C2H8N2	000624-80-6	9
4	Formamide	45	CH3NO	000075-12-7	4
5	4-Penten-2-ol	86	C5H10O	000625-31-0	4





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Data File : VN079521.D
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Operator : JC\MD
Sample : 04823-06
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

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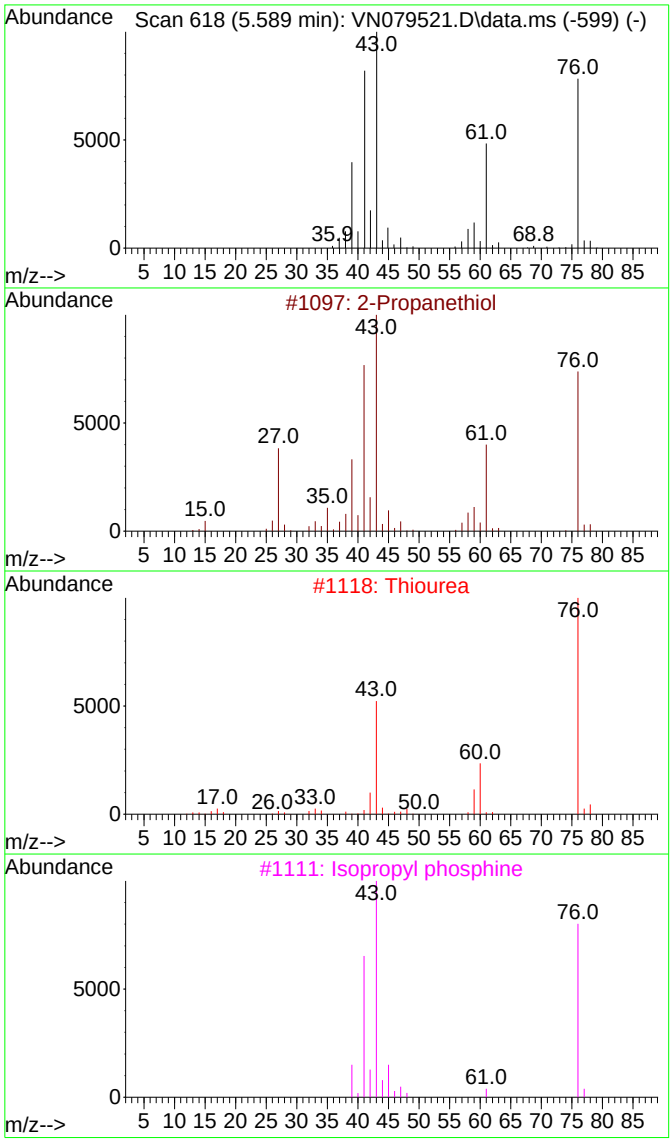
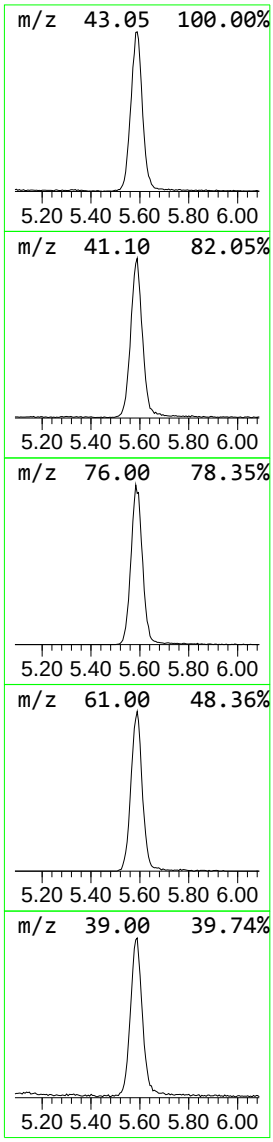
Peak Number 4 2-Propanethiol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.589	48.33 ug/l	1491770	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanethiol	76	C3H8S	000075-33-2	93
2	Thiourea	76	CH4N2S	000062-56-6	59
3	Isopropyl phosphine	76	C3H9P	004538-29-8	45
4	Propyl mercaptan	76	C3H8S	000107-03-9	9
5	Propane, 1,3-dichloro-	112	C3H6Cl2	000142-28-9	9





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Data File : VN079521.D
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Operator : JC\MD
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ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

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

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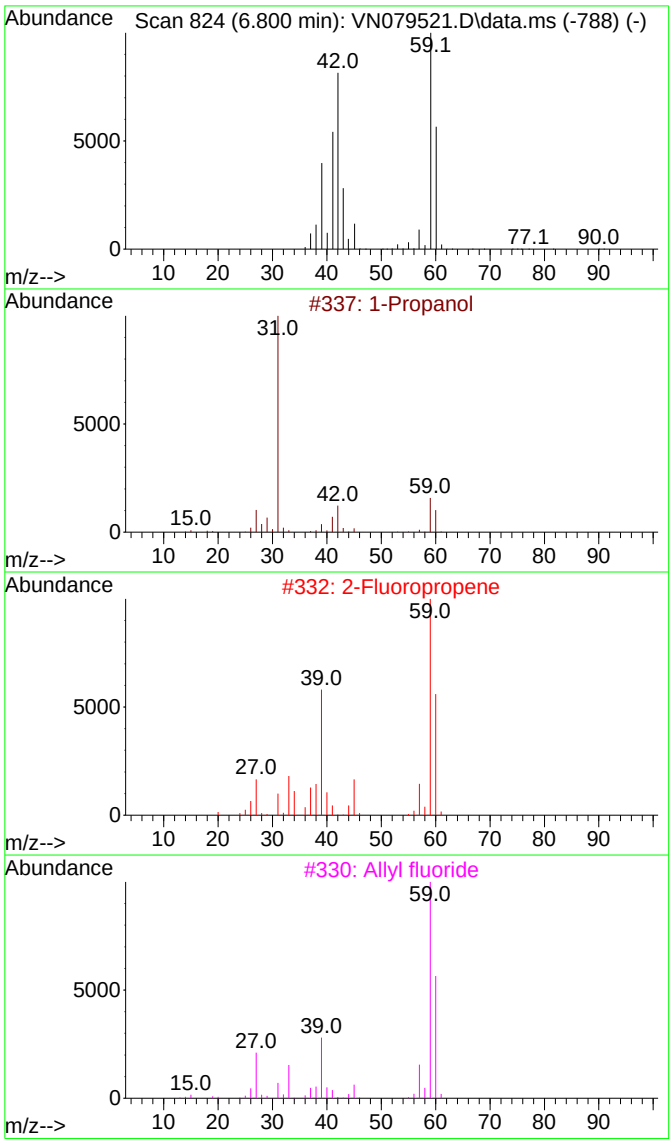
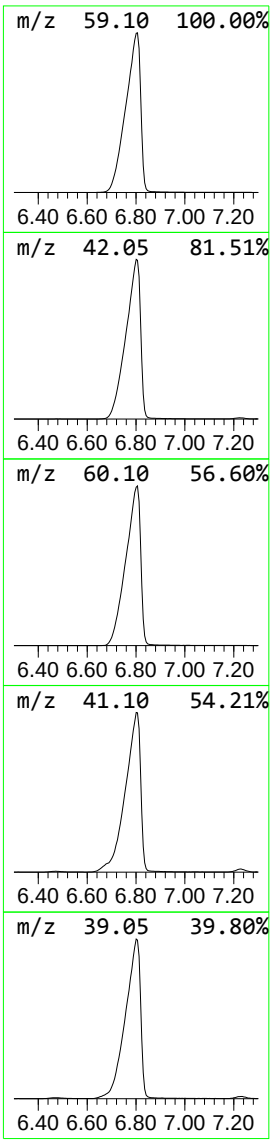
Peak Number 5 1-Propanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.800	1966.36 ug/l	60697600	Pentafluorobenzene	8.230

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol	60	C3H8O	000071-23-8	64
2	2-Fluoropropene	60	C3H5F	001184-60-7	50
3	Allyl fluoride	60	C3H5F	000818-92-8	38
4	Cyclopropane	42	C3H6	000075-19-4	32
5	Formamidoxime	60	CH4N2O	000624-82-8	9





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Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

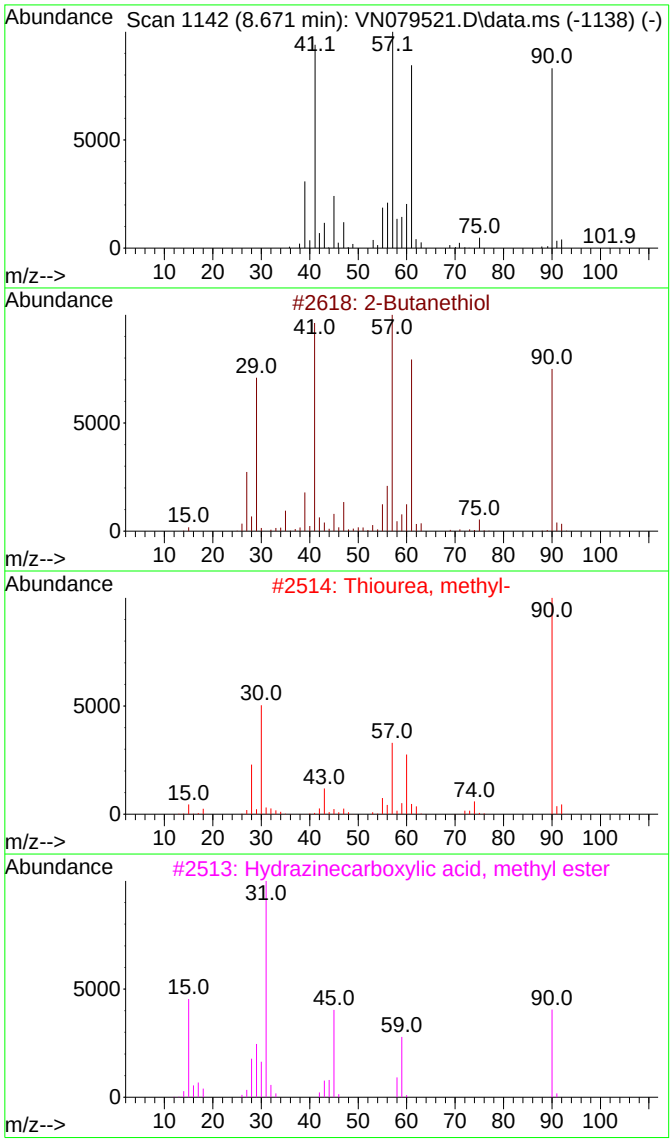
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

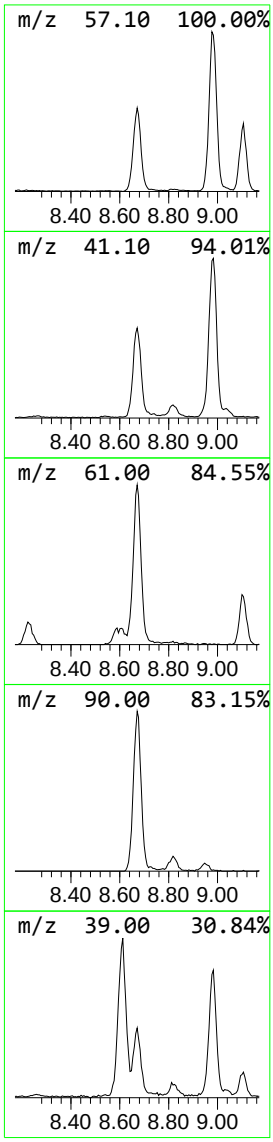
****

Peak Number 6 2-Butanethiol Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.671	15.46 ug/l	661448	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanethiol	90	C4H10S	000513-53-1	90
2	Thiourea, methyl-	90	C2H6N2S	000598-52-7	53
3	Hydrazinecarboxylic acid, methyl...	90	C2H6N2O2	006294-89-9	38
4	(S)-Methyl 2,3-dihydroxypropanoate	120	C4H8O4	010303-88-5	38
5	Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	9





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Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

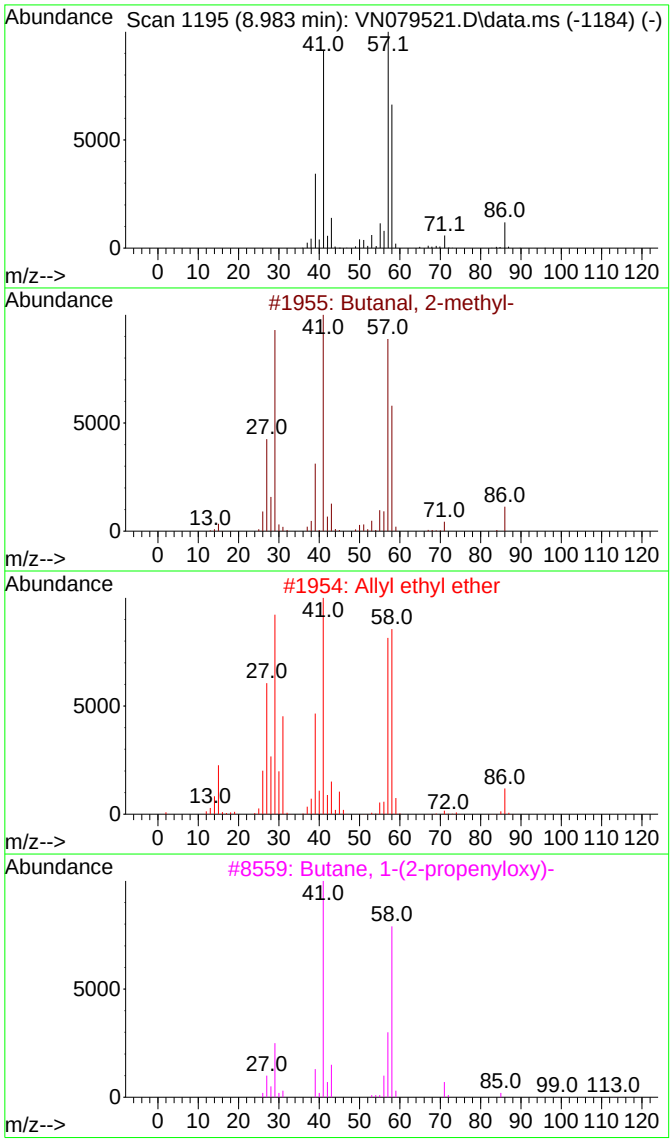
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

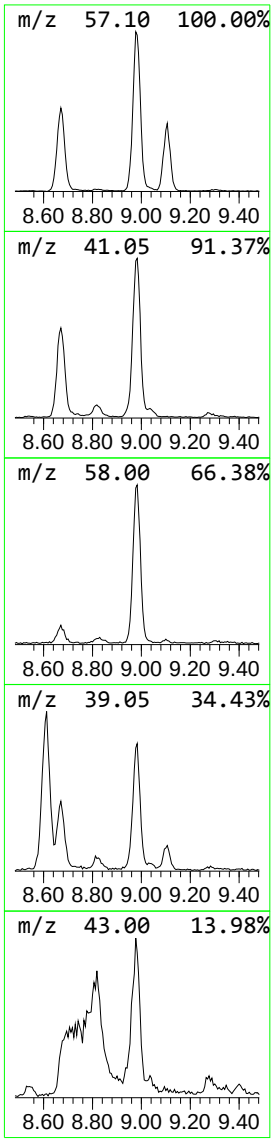
****

Peak Number 7 Butanal, 2-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.983	21.47 ug/l	918622	1,4-Difluorobenzene	9.106

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal, 2-methyl-	86	C5H10O	000096-17-3	90
2	Allyl ethyl ether	86	C5H10O	000557-31-3	50
3	Butane, 1-(2-propenyloxy)-	114	C7H14O	003739-64-8	37
4	2-Penten-1-ol, (E)-	86	C5H10O	001576-96-1	35
5	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	25





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Instrument :
MSVOA_N
ClientSampleId :
TOTES-3

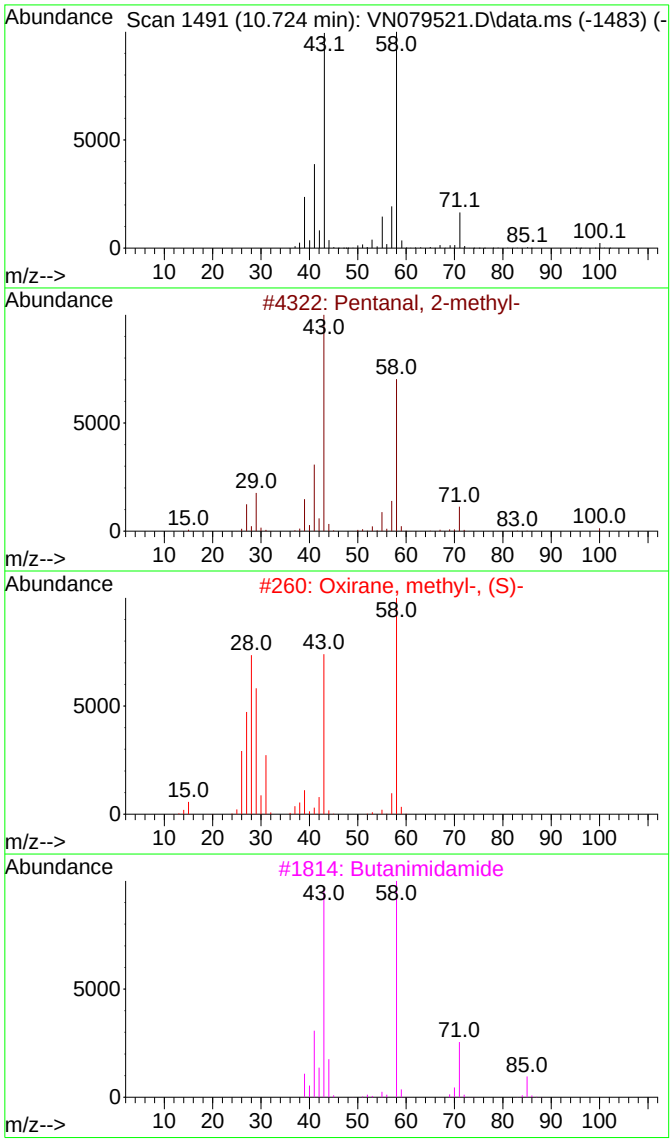
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

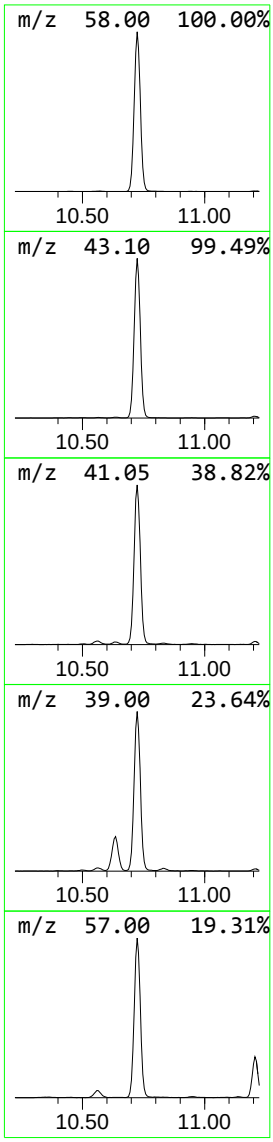
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Pentanal, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.724	286.72 ug/l	15199900	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal, 2-methyl-	100	C6H12O	000123-15-9	91
2	Oxirane, methyl-, (S)-	58	C3H6O	016088-62-3	64
3	Butanimidamide	86	C4H10N2	000107-90-4	56
4	2-Hexanone	100	C6H12O	000591-78-6	39
5	Cyclopropyl methyl carbinol	86	C5H10O	000765-42-4	39





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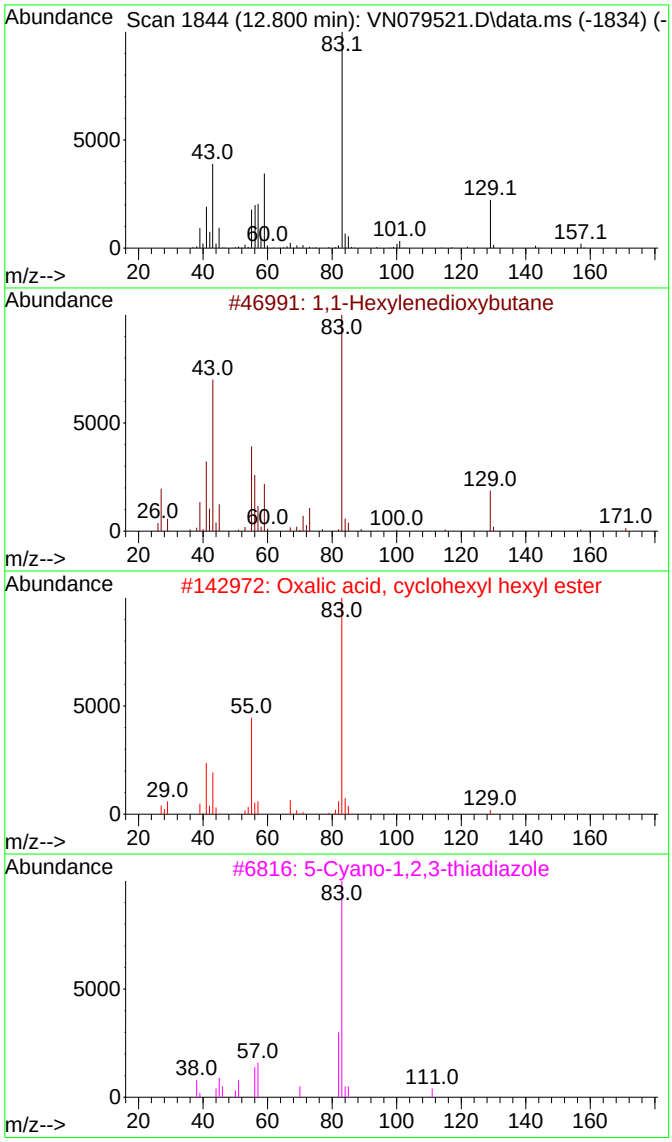
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100523W.M
Quant Title : SW846 8260

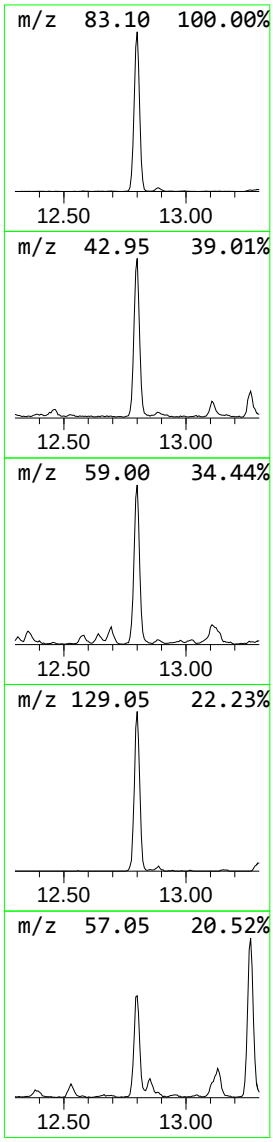
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 1,1-Hexylenedioxybutane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.800	26.06 ug/l	1381530	Chlorobenzene-d5	11.871

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2	Oxalic acid, cyclohexyl hexyl ester	256	C14H24O4	1000309-30-8	43
3	5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	42
4	2-(1-Phenylethyl)-6-isopropyl-1,...	234	C15H22O2	1000431-40-0	36
5	sec-Butyl (E)-2-methylbut-2-enoate	156	C9H16O2	1010373-72-7	33





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TIC Library : C:\Database\NIST20.L
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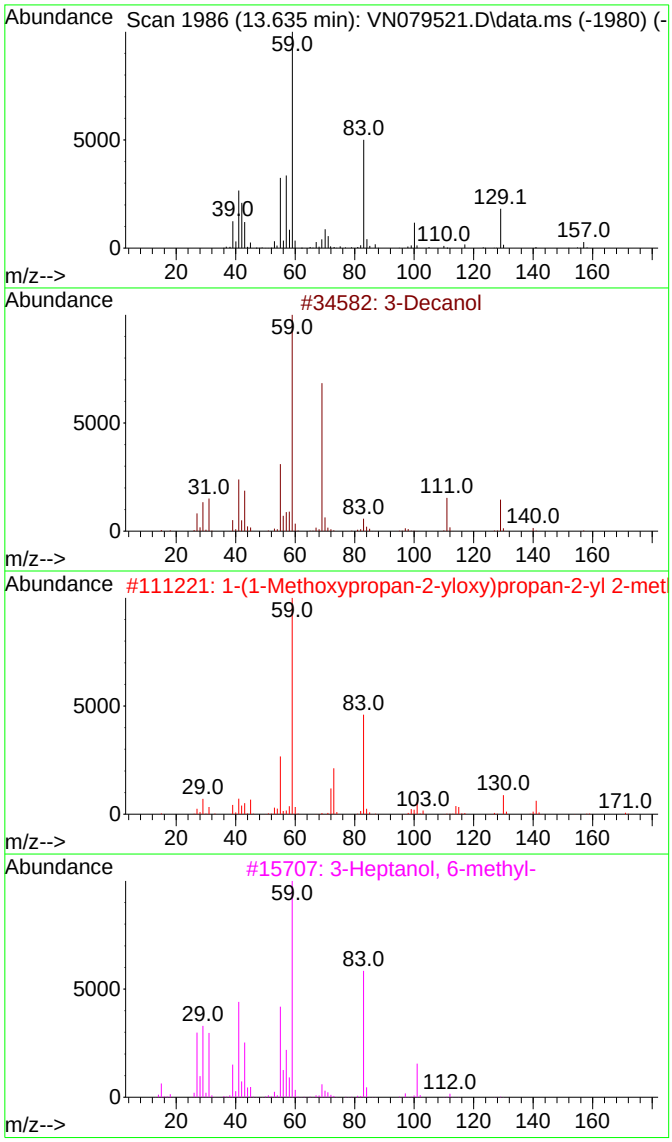
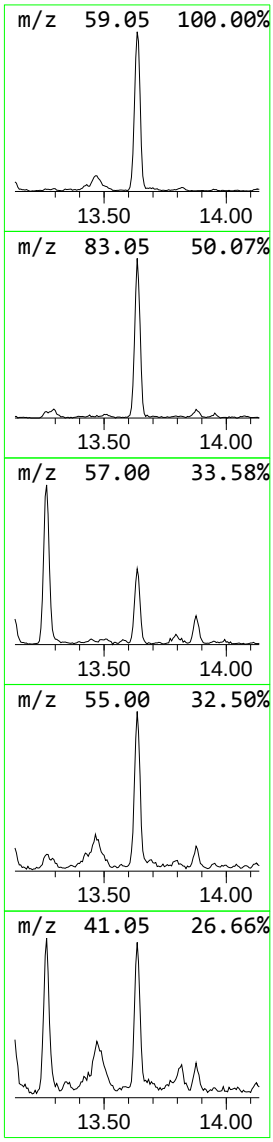
****
Peak Number 10 unknown13.635 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.635	12.39 ug/l	635391	1,4-Dichlorobenzene-d4	13.794

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Decanol	158	C10H22O	001565-81-7	47
2	1-(1-Methoxypropan-2-yloxy)propa...	230	C12H22O4	1000367-11-3	45
3	3-Heptanol, 6-methyl-	130	C8H18O	018720-66-6	42
4	3-Heptanol, 4-methyl-	130	C8H18O	014979-39-6	42
5	Butyl aldoxime, 3-methyl-, anti	101	C5H11NO	005775-74-6	32





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
Isopropyl Alcohol	4.724	24.5	ug/l	755633	1	8.230	1543400	50.0
2-Propanethiol	5.589	48.3	ug/l	1491770	1	8.230	1543400	50.0
1-Propanol	6.800	1966.4	ug/l	60697600	1	8.230	1543400	50.0
2-Butanethiol	8.671	15.5	ug/l	661448	2	9.106	2138880	50.0
Butanal, 2-methyl-	8.983	21.5	ug/l	918622	2	9.106	2138880	50.0
Pentanal, 2-met...	10.724	286.7	ug/l	15199900	3	11.871	2650610	50.0
1,1-Hexylenedio...	12.800	26.1	ug/l	1381530	3	11.871	2650610	50.0
unknown13.635	13.635	12.4	ug/l	635391	4	13.794	2563440	50.0