LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN081525\
Data File : VN087583.D
Acq On : 15 Aug 2025 15:40
Operator : JC\MD
Sample : Q2864-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument : MSVOA_N
ClientSampleId : LAW-25-113-121

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\82N071625W.M
Title : SW846 8260

Signal : TIC: VN087583.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.506	89	94	106	rBV	62904	122959	1.99%	0.628%
2	4.424	410	420	432	rVB	61583	201172	3.25%	1.027%
3	8.153	1044	1054	1058	rBV2	238121	566734	9.16%	2.894%
4	8.212	1058	1064	1076	rVB	375647	869090	14.05%	4.438%
5	8.565	1111	1124	1136	rBV	277885	636364	10.29%	3.250%
6	9.082	1203	1212	1223	rBV	680294	1397105	22.58%	7.134%
7	10.547	1451	1461	1470	rBV	942935	1737787	28.09%	8.874%
8	11.847	1669	1682	1694	rBV	956913	1721332	27.82%	8.790%
9	11.941	1694	1698	1705	rVV	45056	84531	1.37%	0.432%
10	12.047	1708	1716	1725	rVV2	136921	272409	4.40%	1.391%
11	12.376	1765	1772	1782	rBV2	85457	155881	2.52%	0.796%
12	12.829	1840	1849	1862	rBV	654062	1169597	18.91%	5.973%
13	13.641	1982	1987	1995	rBV3	144039	243352	3.93%	1.243%
14	13.770	2001	2009	2019	rBV	955639	1637851	26.47%	8.364%
15	15.647	2319	2328	2333	rBV2	110231	232759	3.76%	1.189%
16	15.717	2333	2340	2348	rVV	603551	1160155	18.75%	5.924%
17	15.811	2348	2356	2365	rVB	572167	1187294	19.19%	6.063%
18	16.000	2379	2388	2431	rBV	1685285	6186661	100.00%	31.592%

Sum of corrected areas: 19583033

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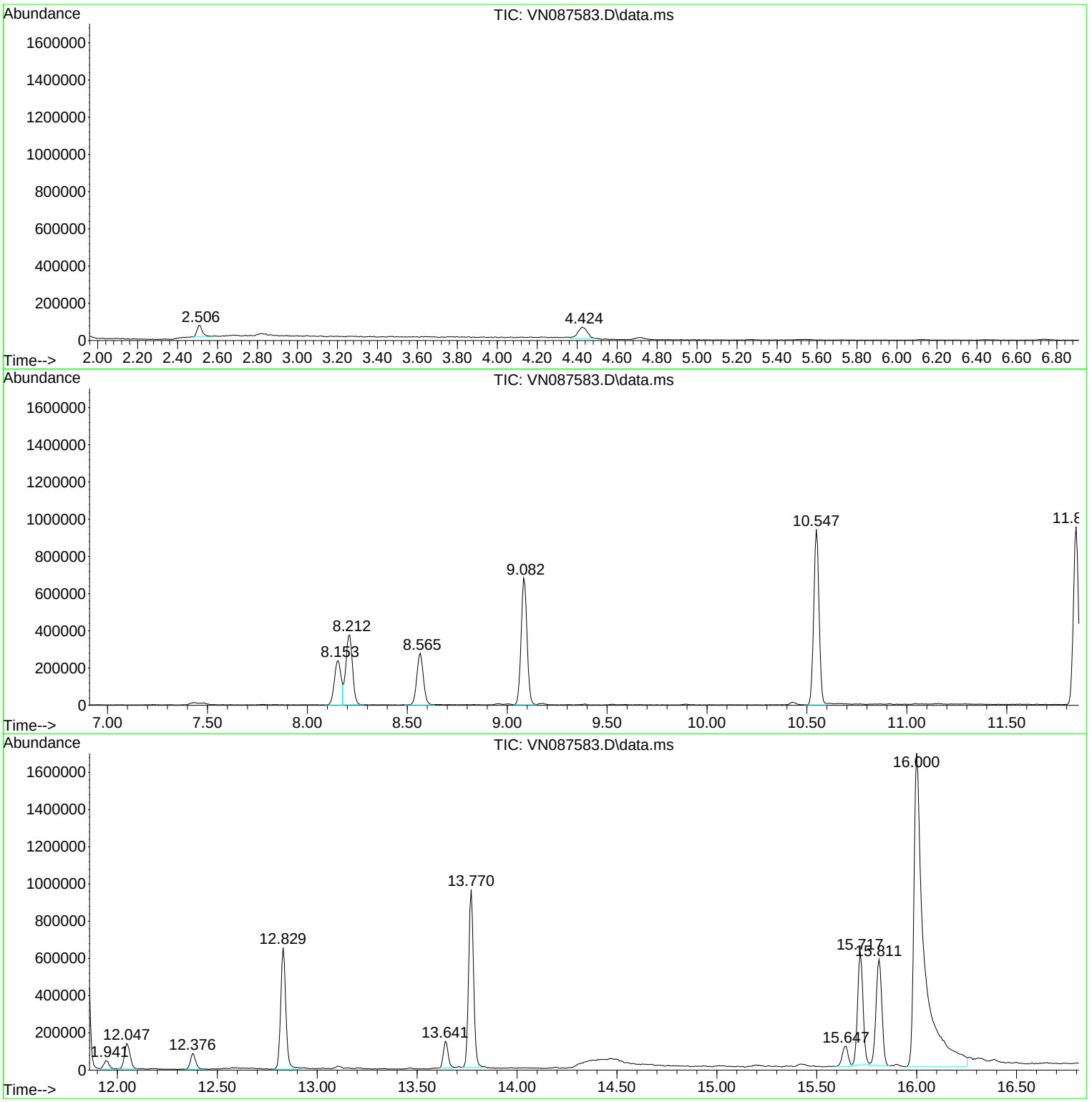
ClientSampleId :
LAW-25-113-121

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

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



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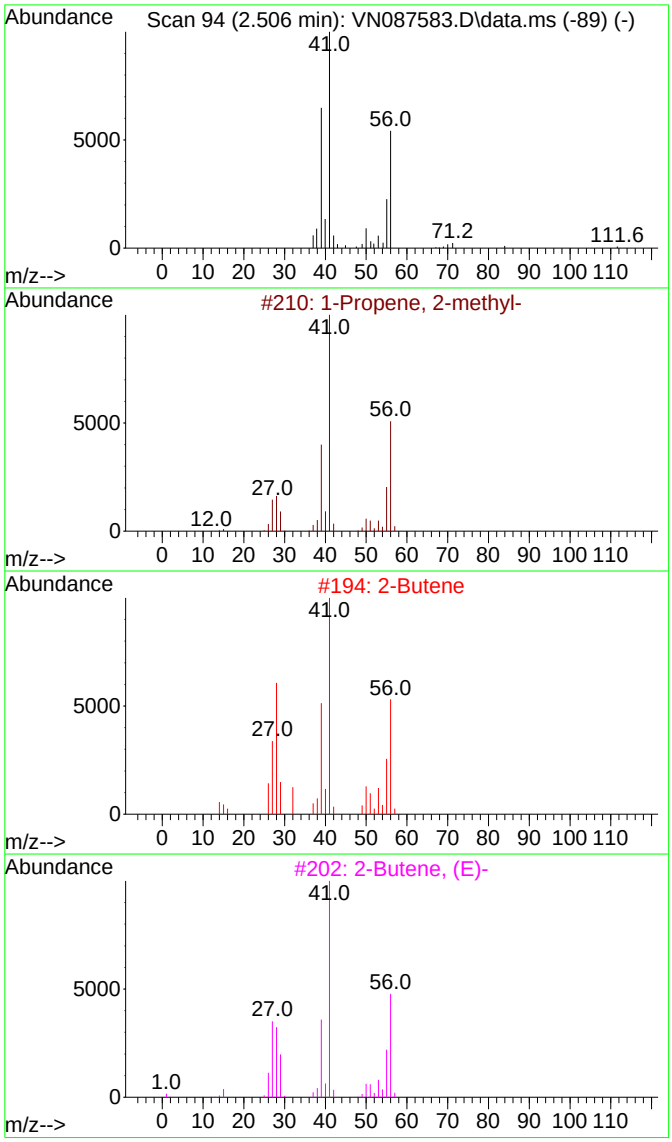
Quant Title : SW846 8260

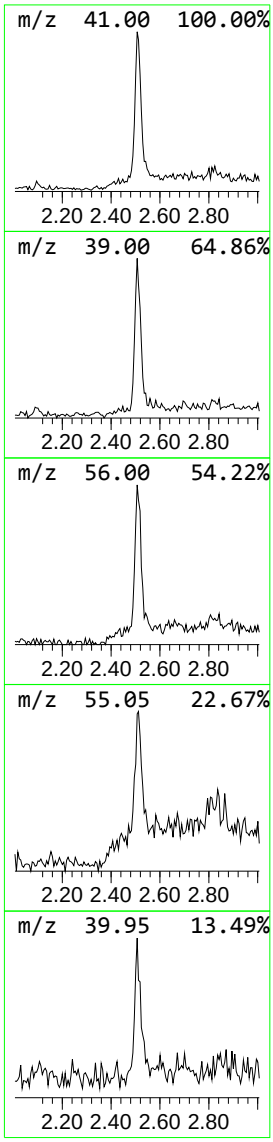
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 1-Propene, 2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.506	7.07 ug/l	122959	Pentafluorobenzene	8.212

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 2-methyl-	56	C4H8	000115-11-7	87
2	2-Butene	56	C4H8	000107-01-7	80
3	2-Butene, (E)-	56	C4H8	000624-64-6	47
4	2-Butene, (Z)-	56	C4H8	000590-18-1	47
5	1-Butene	56	C4H8	000106-98-9	46





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ClientSampleId :
LAW-25-113-121

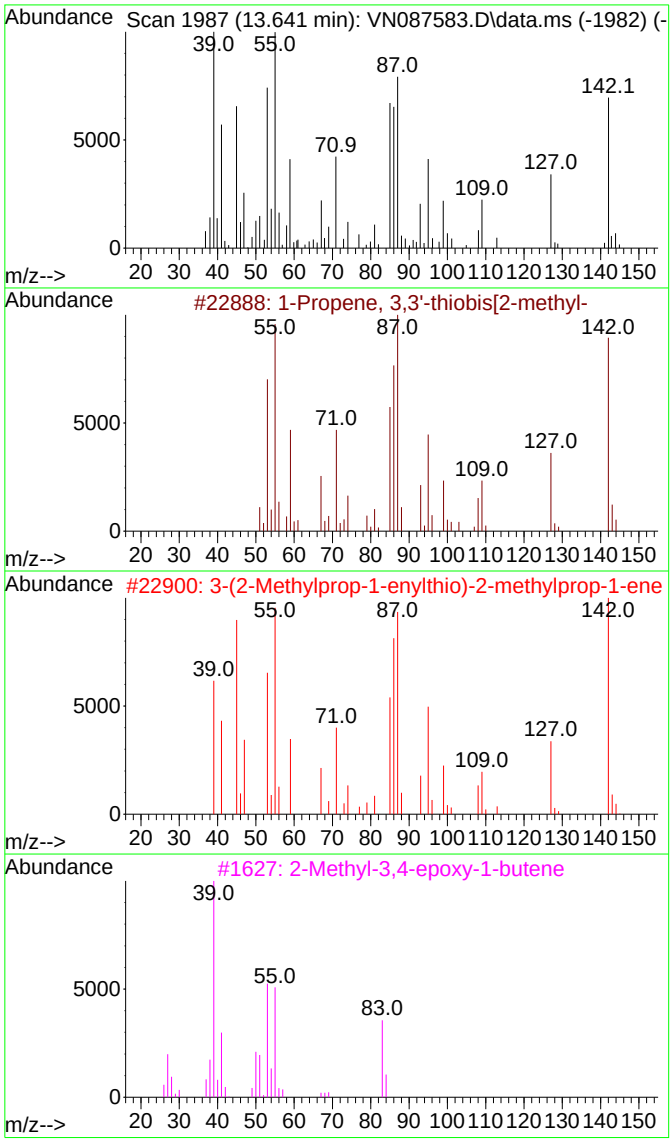
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

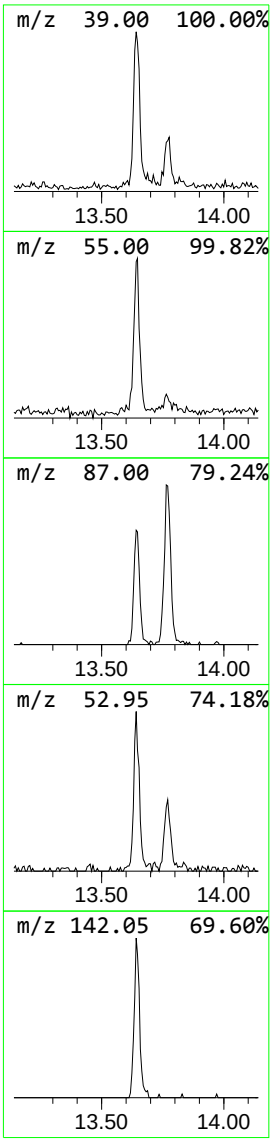
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1-Propene, 3,3'-thiobis[2-m... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.641	7.43 ug/l	243352	1,4-Dichlorobenzene-d4	13.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propene, 3,3'-thiobis[2-methyl-	142	C8H14S	023973-54-8	94
2	3-(2-Methylprop-1-enylthio)-2-me...	142	C8H14S	1000122-39-8	93
3	2-Methyl-3,4-epoxy-1-butene	84	C5H8O	1000432-31-7	40
4	2-Ethylprop-1-ene (1-3)sultine	132	C5H8O2S	084735-13-7	36
5	3,4-Pentadienal	82	C5H6O	004009-55-6	32





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Instrument :
MSVOA_N
ClientSampleId :
LAW-25-113-121

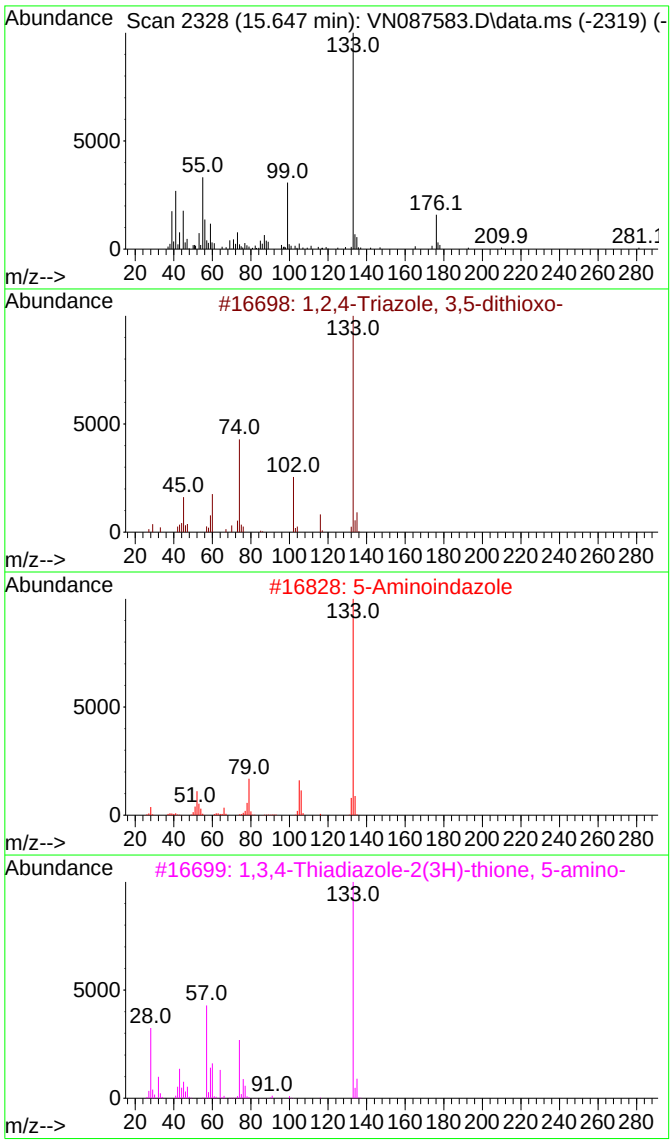
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

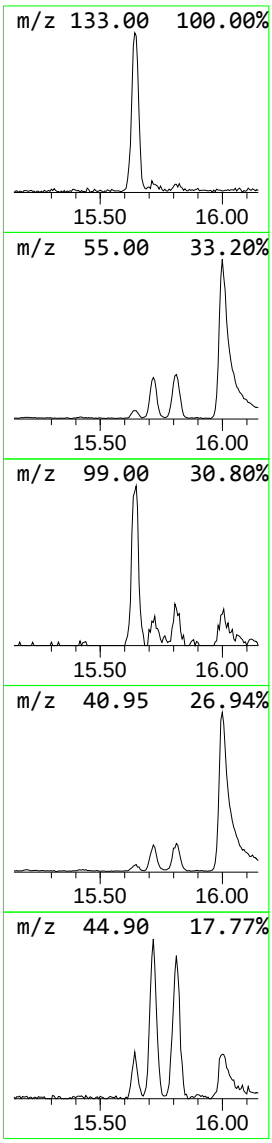
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 1,2,4-Triazole, 3,5-dithioxo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.647	7.11 ug/l	232759	1,4-Dichlorobenzene-d4	13.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	50
2	5-Aminoindazole	133	C7H7N3	019335-11-6	43
3	1,3,4-Thiadiazole-2(3H)-thione, ...	133	C2H3N3S2	002349-67-9	40
4	(2-Methyl[1,3]dithian-2-yl)methanol	164	C6H12OS2	1000191-37-4	38
5	1-Propanone, 2-chloro-1-(4-ethyl...	210	C12H15ClO	055012-69-6	37





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Instrument :
MSVOA_N
ClientSampleId :
LAW-25-113-121

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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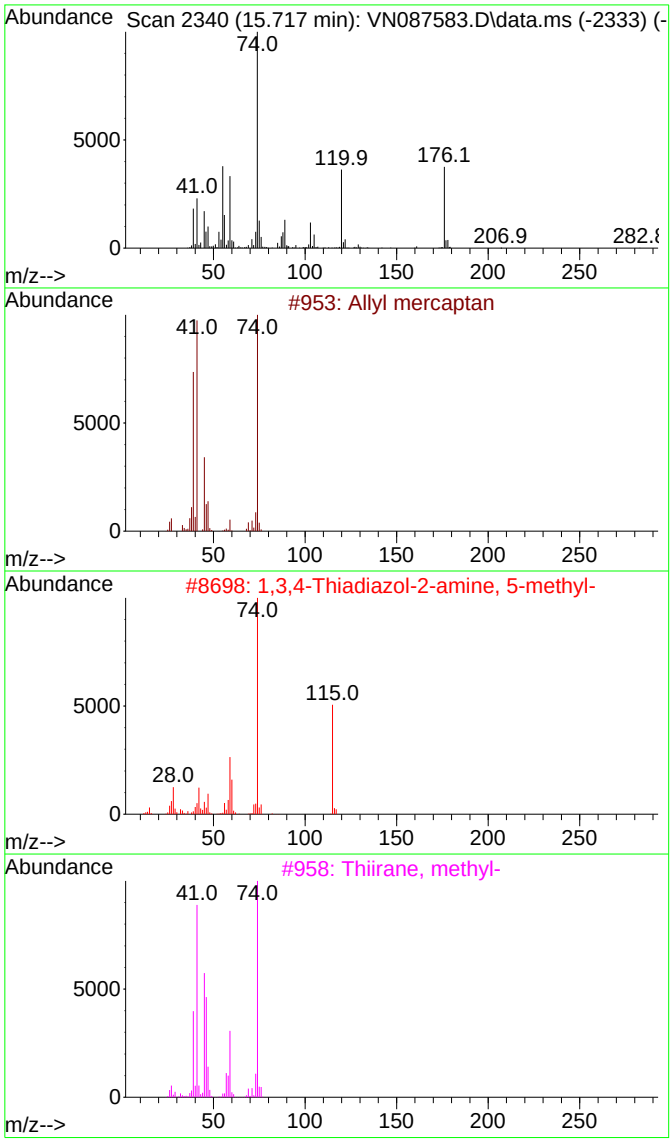
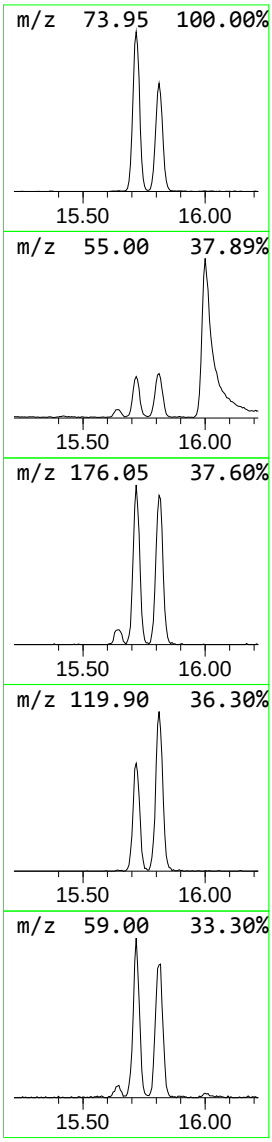
****

Peak Number 4 unknown15.717 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.717	35.42 ug/l	1160160	1,4-Dichlorobenzene-d4	13.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Allyl mercaptan	74	C3H6S	000870-23-5	46
2	1,3,4-Thiadiazol-2-amine, 5-methyl-	115	C3H5N3S	000108-33-8	38
3	Thiirane, methyl-	74	C3H6S	001072-43-1	38
4	2-Propenoic acid, 2-(methylthio)...	146	C6H10O2S	004836-09-3	37
5	dl-Homoserine	119	C4H9NO3	001927-25-9	35





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MSVOA_N
ClientSampleId :
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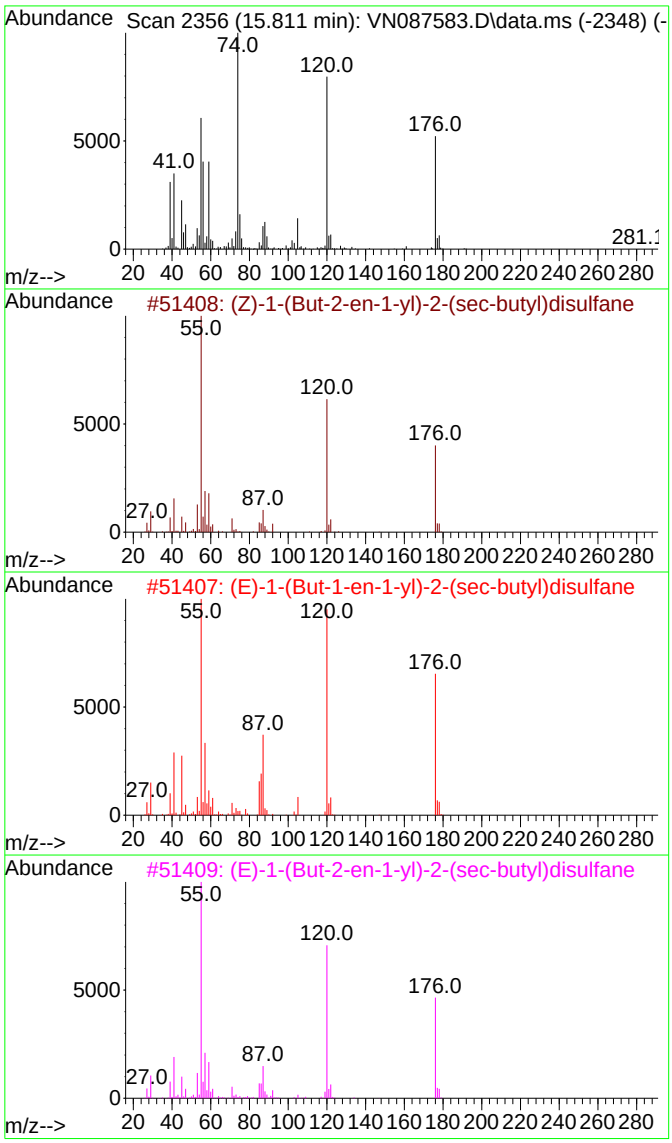
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N071625W.M
Quant Title : SW846 8260

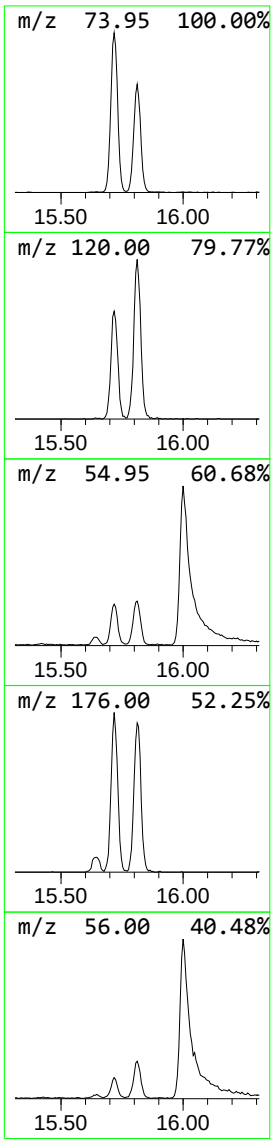
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 unknown15.812 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.812	36.25 ug/l	1187290	1,4-Dichlorobenzene-d4	13.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(Z)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-23-8	42
2	(E)-1-(But-1-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-22-7	38
3	(E)-1-(But-2-en-1-yl)-2-(sec-but...	176	C8H16S2	110690-24-9	38
4	Disulfide, methyl 2-propenyl	120	C4H8S2	002179-58-0	30
5	dl-Homoserine	119	C4H9NO3	001927-25-9	30





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Quant Title : SW846 8260

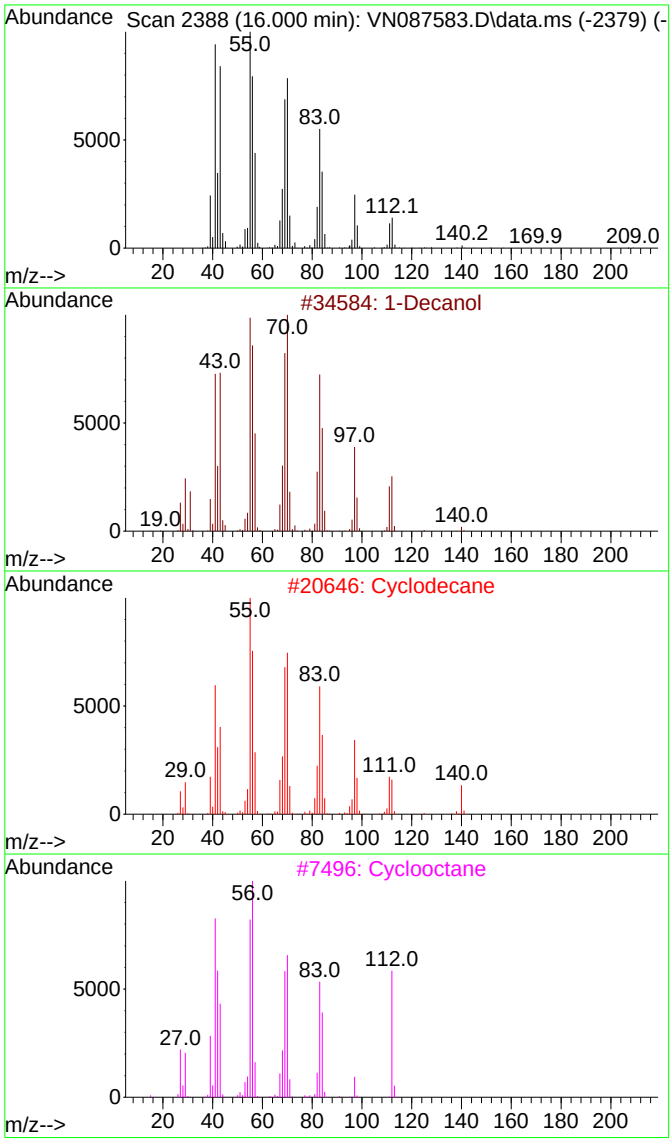
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

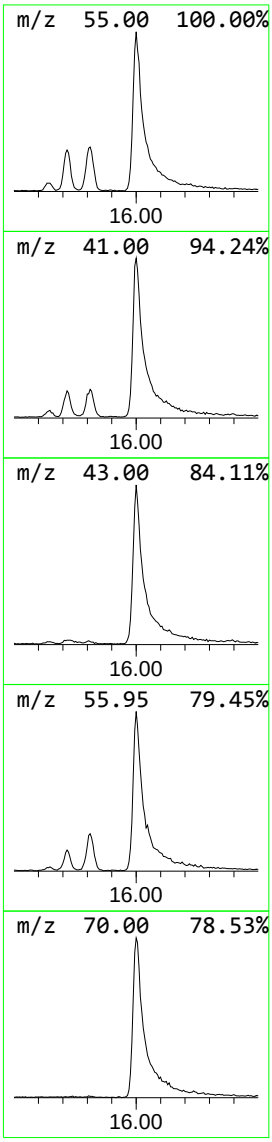
****

Peak Number 6 1-Decanol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.000	188.87 ug/l	6186660	1,4-Dichlorobenzene-d4	13.770

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Decanol	158	C10H22O	000112-30-1	91
2	Cyclodecane	140	C10H20	000293-96-9	87
3	Cyclooctane	112	C8H16	000292-64-8	87
4	Formic acid, decyl ester	186	C11H22O2	005451-52-5	86
5	1-Undecanol	172	C11H24O	000112-42-5	86





Tentatively Identified Compound (LSC) summary

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TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
1-Propene, 2-me...	2.506	7.1	ug/l	122959	1	8.212	869090	50.0
1-Propene, 3,3'...	13.641	7.4	ug/l	243352	4	13.770	1637850	50.0
1,2,4-Triazole,...	15.647	7.1	ug/l	232759	4	13.770	1637850	50.0
unknown15.717	15.717	35.4	ug/l	1160160	4	13.770	1637850	50.0
unknown15.812	15.812	36.3	ug/l	1187290	4	13.770	1637850	50.0
1-Decanol	16.000	188.9	ug/l	6186660	4	13.770	1637850	50.0