LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU101419\
Data File : VU035145.D
Acq On : 14 Oct 2019 12:18
Operator : JC/SP
Sample : K5309-18
Misc : 25.0mL/MSVOA U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RD-9-001-01

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.1 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_U\METHOD\SOMUTR100719WMA.M
Title : TRACE VOA SOM01.0

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.174	19	26	50	rBV	5702831	5752351	100.00%	43.716%
2	1.395	85	95	111	rBV	721818	792277	13.77%	6.021%
3	1.672	174	181	198	rVB	66597	93515	1.63%	0.711%
4	2.260	355	364	376	rBV	117363	172615	3.00%	1.312%
5	2.961	569	582	606	rBV	551582	1029748	17.90%	7.826%
6	4.196	948	966	1010	rVB3	183006	613611	10.67%	4.663%
7	4.624	1084	1099	1125	rVB	88510	224647	3.91%	1.707%
8	5.315	1289	1314	1348	rBV2	183708	528705	9.19%	4.018%
9	5.865	1472	1485	1508	rBV	195865	399384	6.94%	3.035%
10	6.312	1610	1624	1645	rBV	130246	262061	4.56%	1.992%
11	7.212	1889	1904	1924	rBV2	52526	104511	1.82%	0.794%
12	7.546	1995	2008	2024	rBV	220122	397883	6.92%	3.024%
13	7.836	2087	2098	2124	rBV	30288	62233	1.08%	0.473%
14	8.299	2229	2242	2284	rBV	266359	608241	10.57%	4.622%
15	9.070	2470	2482	2522	rBV2	301947	649569	11.29%	4.936%
16	10.231	2830	2843	2885	rBV	189847	351705	6.11%	2.673%
17	10.414	2889	2900	2919	rBV	104562	178766	3.11%	1.359%
18	11.466	3216	3227	3252	rBV	251831	464491	8.07%	3.530%
19	11.842	3329	3344	3366	rBV	202673	370977	6.45%	2.819%
20	13.048	3708	3719	3744	rBV2	52902	101211	1.76%	0.769%

Sum of corrected areas: 13158501

LSC Report - Integrated Chromatogram

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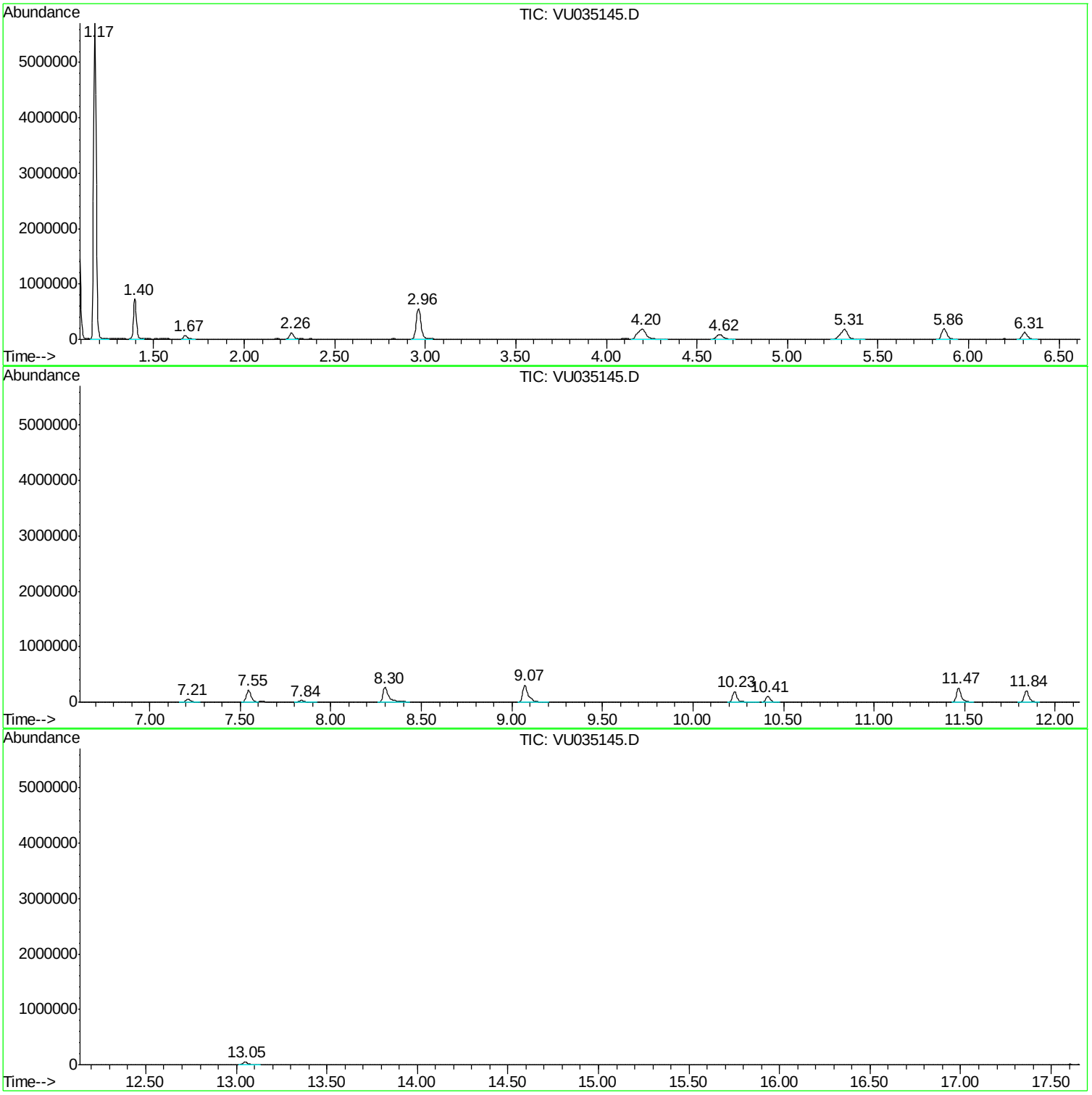
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100719WMA.M
Quant Title : TRACE VOA SOM01.0

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



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

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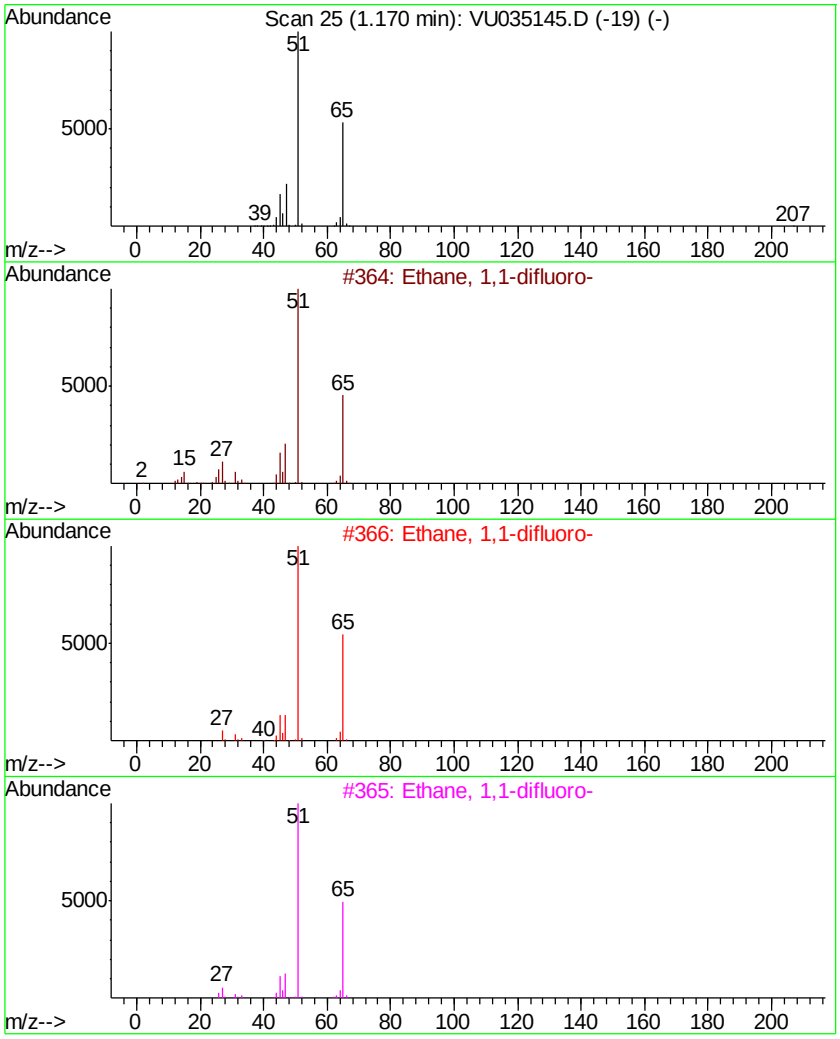
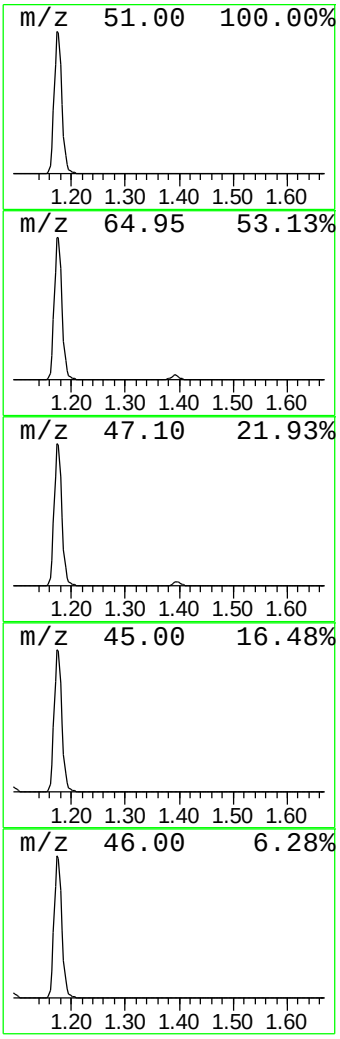
Peak Number 1 Ethane, 1,1-difluoro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.17	72.02 ug/L	5752350	1,4-Difluorobenzene	5.86

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
2	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	91
3	Ethane, 1,1-difluoro-	66	C2H4F2	000075-37-6	90
4	Propiolonitrile	51	C3HN	001070-71-9	3
5	Propane, 2,2-difluoro-	80	C3H6F2	000420-45-1	2





Library Search Compound Report

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ClientSampleId : RD-9-001-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100719WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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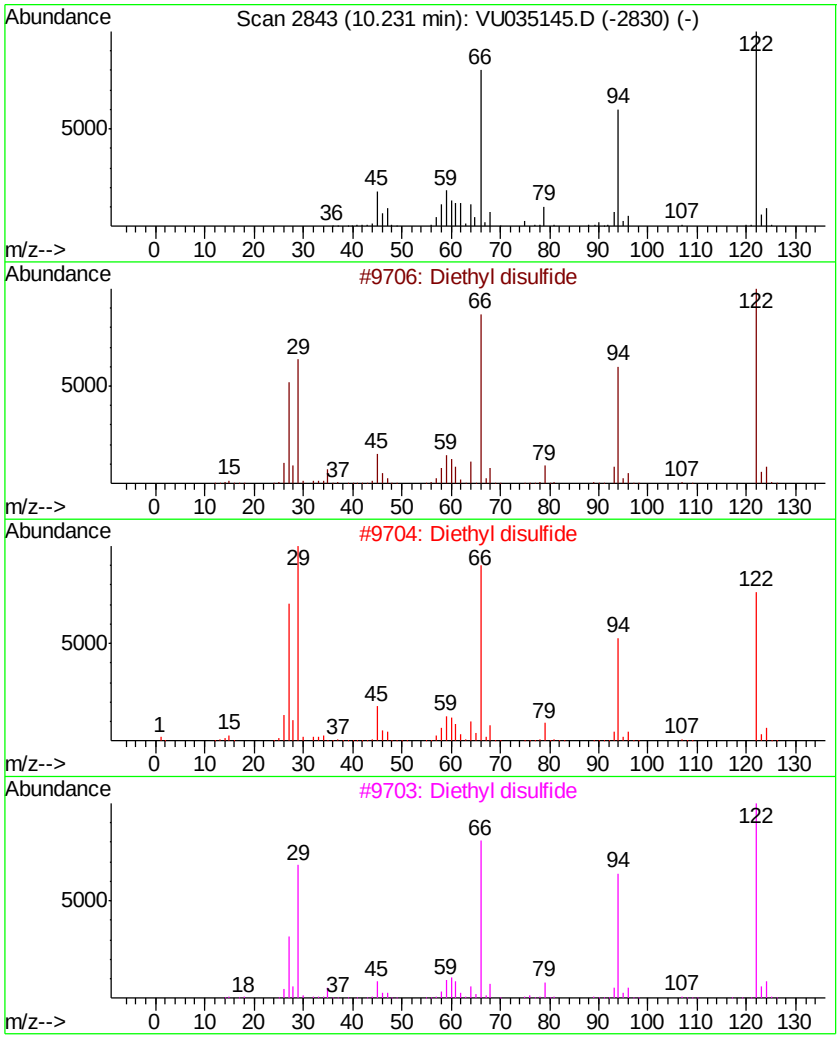
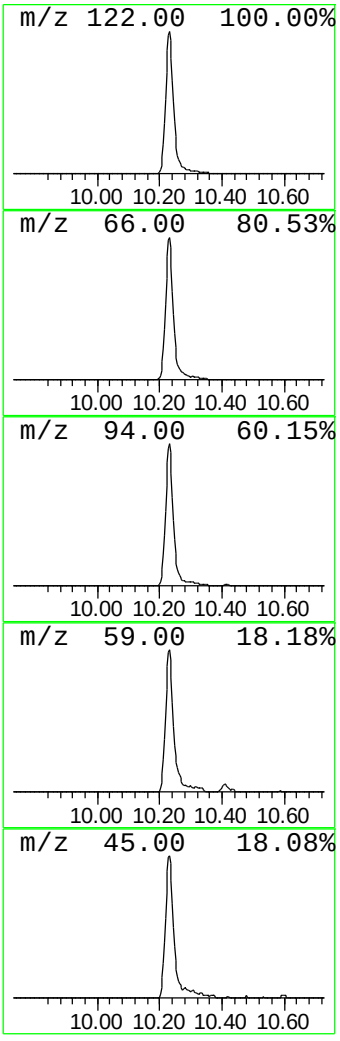
Peak Number 3 Diethyl disulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.23	2.71 ug/L	351705	Chlorobenzene-d5	9.07

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethyl disulfide	122	C4H10S2	000110-81-6	94
2	Diethyl disulfide	122	C4H10S2	000110-81-6	90
3	Diethyl disulfide	122	C4H10S2	000110-81-6	90
4	6-exo-Methyl-5-exo-norbornenol	124	C8H12O	060362-83-6	47
5	5-exo-Methyl-5-norbornenol	124	C8H12O	003212-13-3	38





Library Search Compound Report

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ALS Vial : 7 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : RD-9-001-01

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMUTR100719WMA.M
Quant Title : TRACE VOA SOM01.0

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

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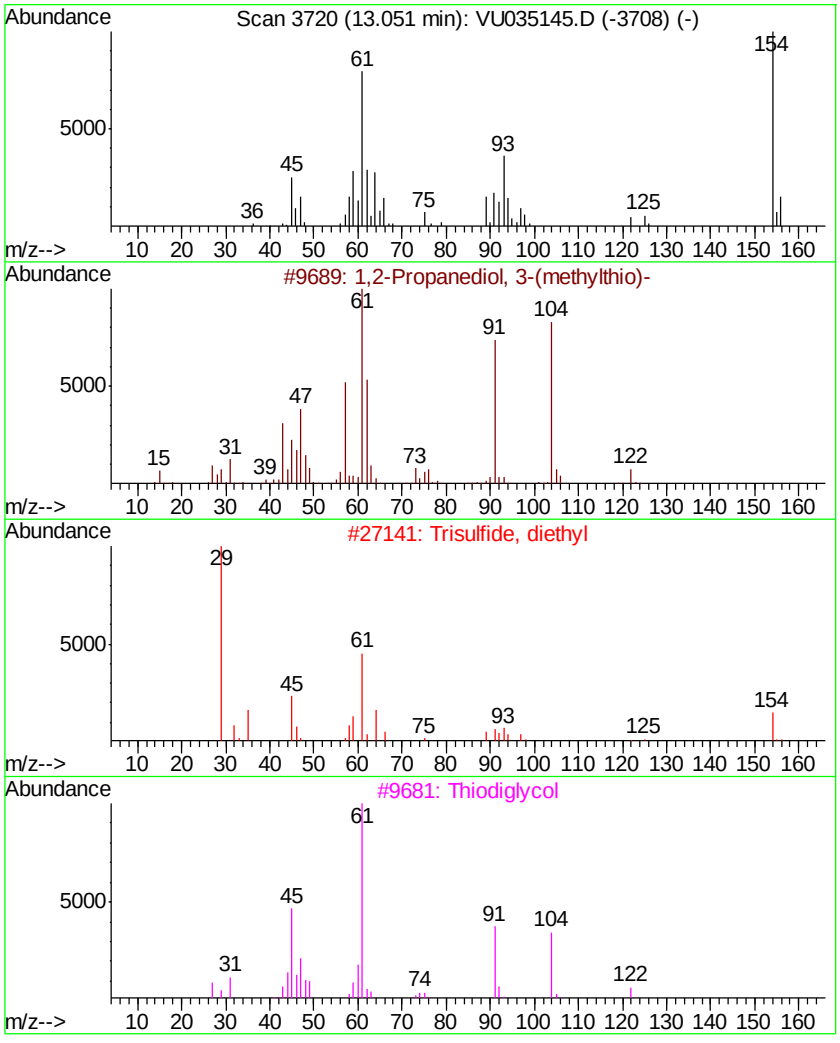
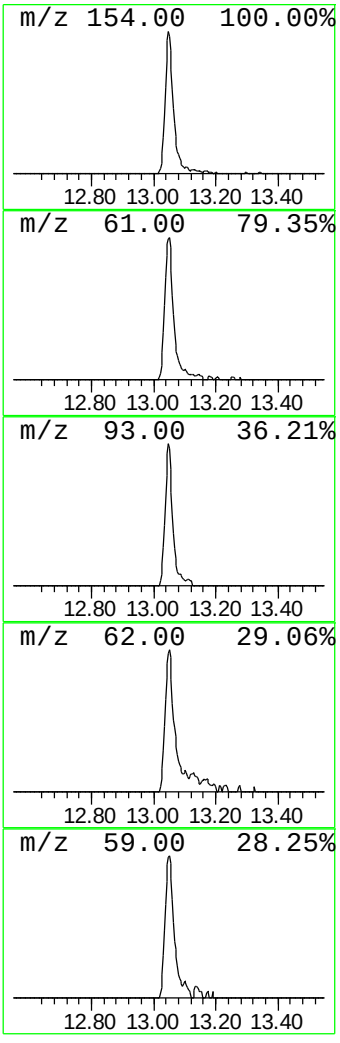
Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.05	1.09 ug/L	101211	1,4-Dichlorobenzene-d4	11.47

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,2-Propanediol, 3-(methylthio)-	122	C4H10O2S	022551-26-4	27
2	Trisulfide, diethyl	154	C4H10S3	003600-24-6	25
3	Thiodiglycol	122	C4H10O2S	000111-48-8	18
4	5-Chloro-benzofurazan	154	C6H3ClN2O	019155-86-3	16
5	4-Nitro-2-picoline N-oxide	154	C6H6N2O3	005470-66-6	14





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SOM01.0

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Ethane, 1,1-diflu...	1.17	72.0	ug/L	5752350	1	5.86	399384	5.0
Diethyl disulfide	10.23	2.7	ug/L	351705	2	9.07	649569	5.0
unknown-01	13.05	1.1	ug/L	101211	3	11.47	464491	5.0