LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
Data File : VU051728.D
Acq On : 03 Nov 2022 12:54
Operator : JC/MD
Sample : N5301-19
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBWN4

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\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU051728.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.392	10	16	30	rVB2	14541	24064	2.99%	0.347%
2	1.594	40	79	85	rBV	205775	804907	100.00%	11.622%
3	1.784	132	138	155	rVB	349412	465424	57.82%	6.720%
4	2.562	368	380	392	rVB	127736	204537	25.41%	2.953%
5	2.681	406	417	437	rVB2	31284	63637	7.91%	0.919%
6	2.787	441	450	460	rBV	11680	18749	2.33%	0.271%
7	3.829	769	774	790	rVB	4363	8875	1.10%	0.128%
8	4.658	1017	1032	1070	rBV3	67778	265357	32.97%	3.832%
9	5.060	1142	1157	1179	rBV	129793	295598	36.72%	4.268%
10	5.723	1343	1363	1397	rBV2	241457	632963	78.64%	9.140%
11	6.247	1512	1526	1550	rBV	208409	405650	50.40%	5.857%
12	6.543	1609	1618	1627	rBV7	5058	9173	1.14%	0.132%
13	6.690	1648	1664	1679	rVV	158572	321010	39.88%	4.635%
14	6.761	1682	1686	1702	rVB8	6300	13321	1.65%	0.192%
15	7.565	1920	1936	1956	rBV	67716	123629	15.36%	1.785%
16	7.678	1960	1971	1997	rVV2	21175	47611	5.92%	0.687%
17	7.896	2027	2039	2055	rBV	257816	441077	54.80%	6.369%
18	8.179	2117	2127	2139	rBV2	40745	69358	8.62%	1.001%
19	8.472	2208	2218	2238	rBV5	9261	25341	3.15%	0.366%
20	8.636	2258	2269	2300	rBV	278427	611508	75.97%	8.830%
21	8.864	2332	2340	2347	rVB5	7344	11192	1.39%	0.162%
22	9.417	2495	2512	2538	rBV	322973	556326	69.12%	8.033%
23	9.597	2554	2568	2579	rBV3	12159	19624	2.44%	0.283%
24	10.012	2684	2697	2720	rBV6	21794	69426	8.63%	1.002%
25	10.755	2917	2928	2950	rVB	132822	220713	27.42%	3.187%
26	10.890	2961	2970	2982	rVB2	11264	18945	2.35%	0.274%
27	11.362	3106	3117	3130	rBV3	21199	42480	5.28%	0.613%
28	11.809	3244	3256	3273	rBV	324667	522753	64.95%	7.548%
29	12.066	3325	3336	3351	rBV3	14977	31782	3.95%	0.459%
30	12.192	3360	3375	3393	rBV	269500	447112	55.55%	6.456%
31	12.549	3475	3486	3502	rVB10	5061	11388	1.41%	0.164%
32	13.619	3809	3819	3835	rBV5	18672	32421	4.03%	0.468%
33	14.095	3959	3967	3975	rBV5	8015	13001	1.62%	0.188%
34	14.144	3975	3982	3992	rVB6	8504	12663	1.57%	0.183%
35	14.613	4120	4128	4140	rVB4	19820	32509	4.04%	0.469%
36	15.545	4409	4418	4431	rBV6	20025	31387	3.90%	0.453%

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Title : TRACE VOA SFAM1.0

Sum of corrected areas: 6925511

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110322\
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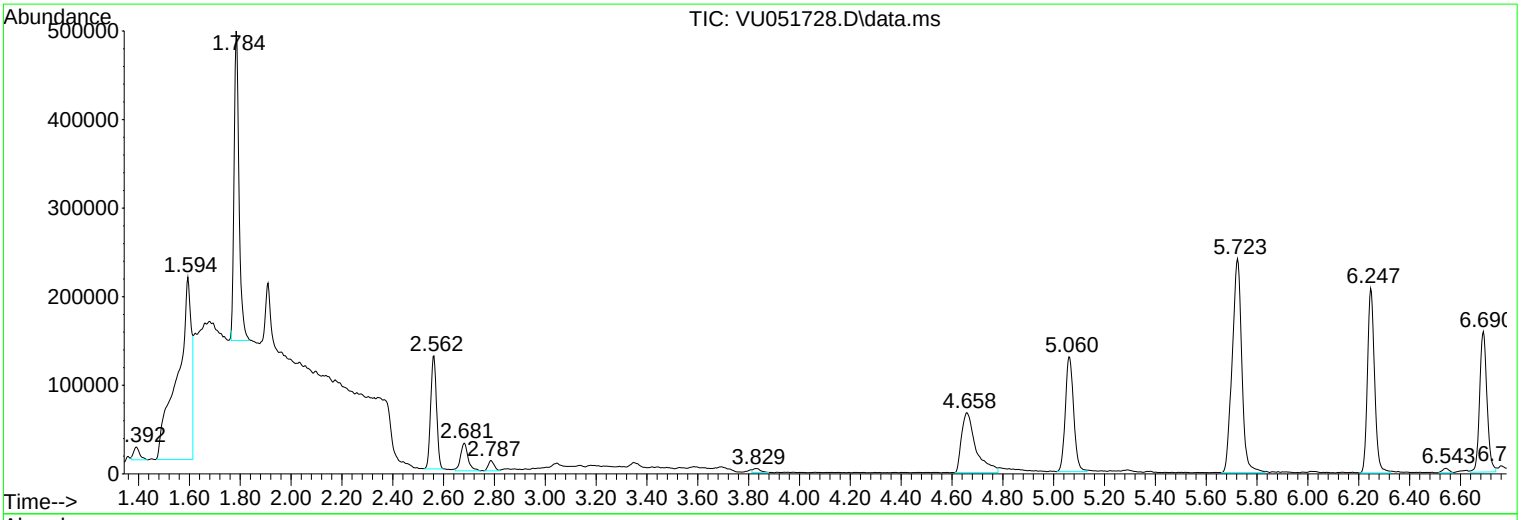
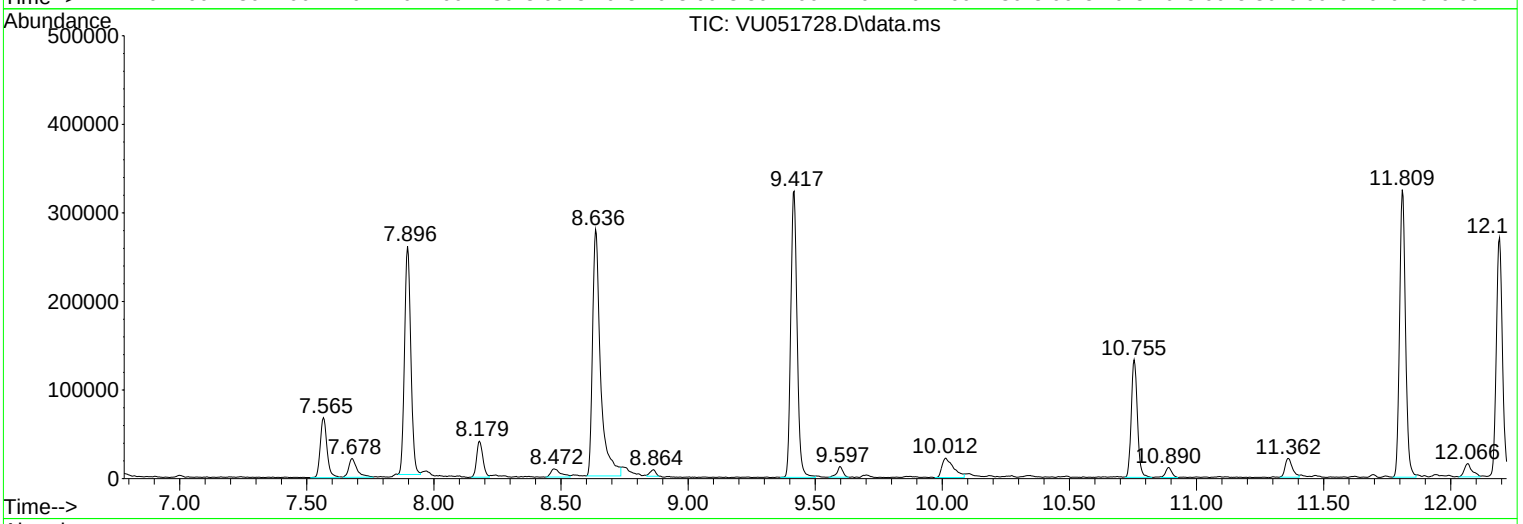
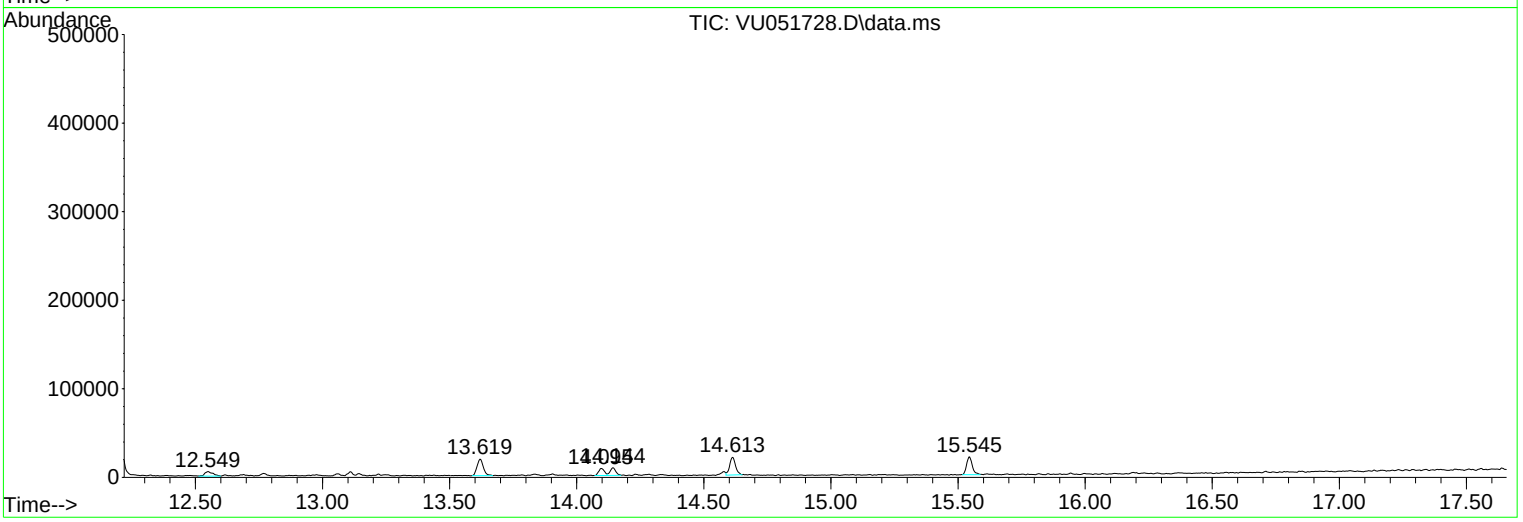
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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







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Quant Title : TRACE VOA SFAM1.0

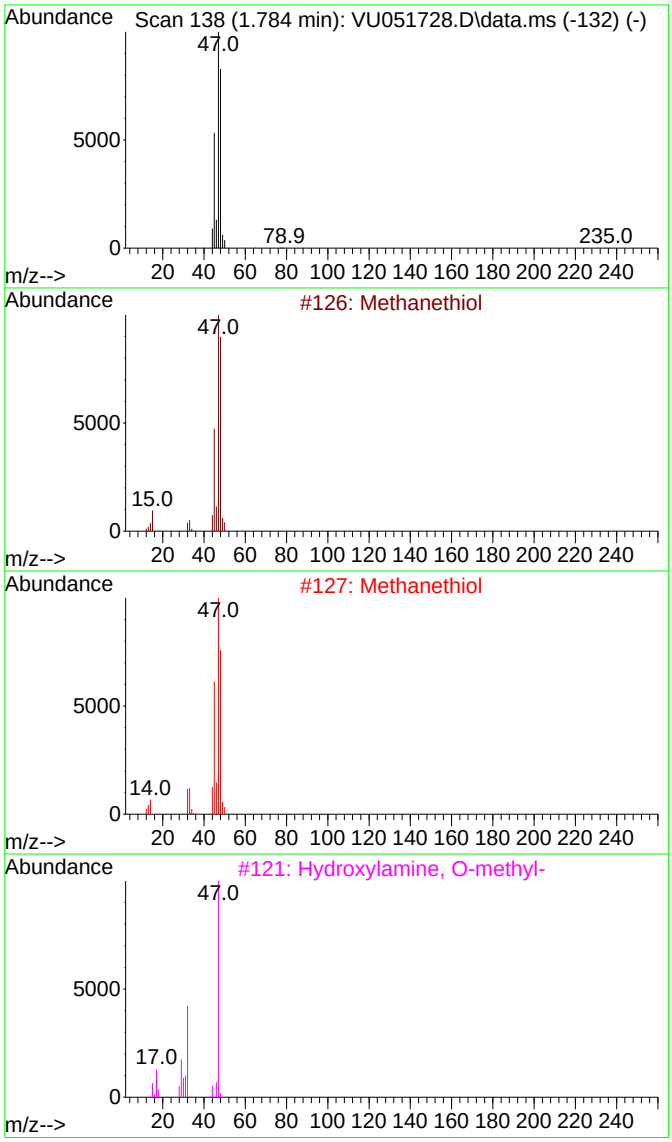
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

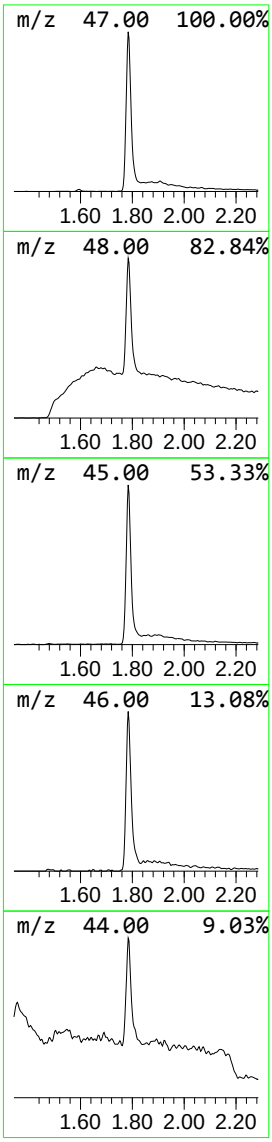
****

Peak Number 1 Methanethiol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.784	5.74 ug/L	465424	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	90
2	Methanethiol	48	CH4S	000074-93-1	86
3	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5	Methane, nitroso-	45	CH3NO	000865-40-7	5





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Instrument :
MSVOA_U
ClientSampleId :
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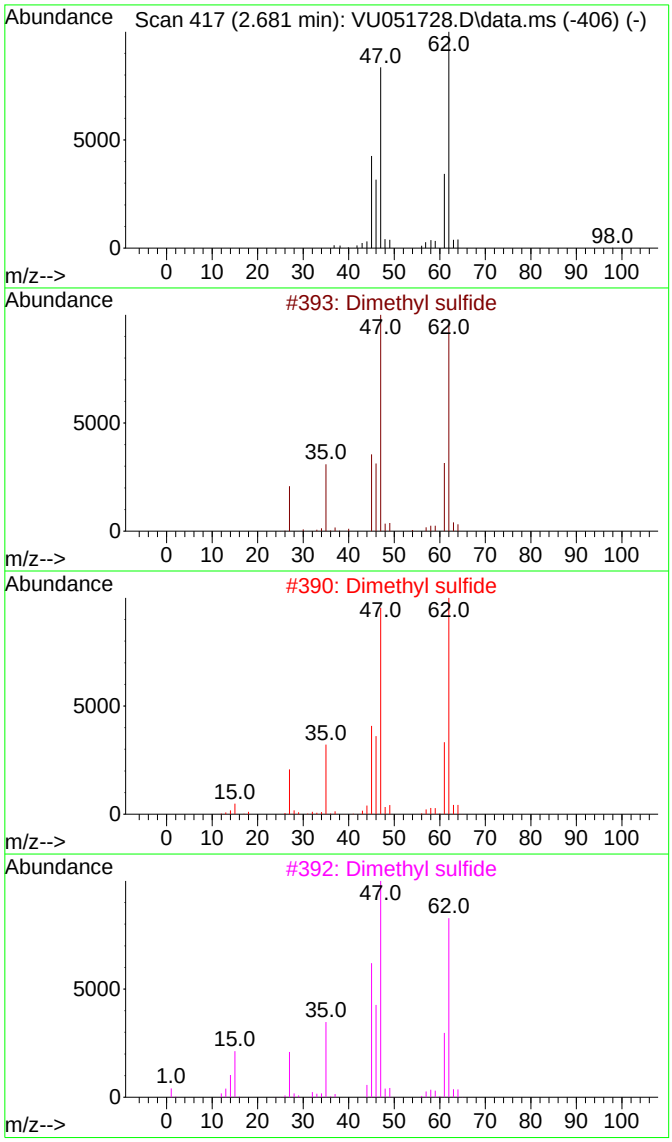
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

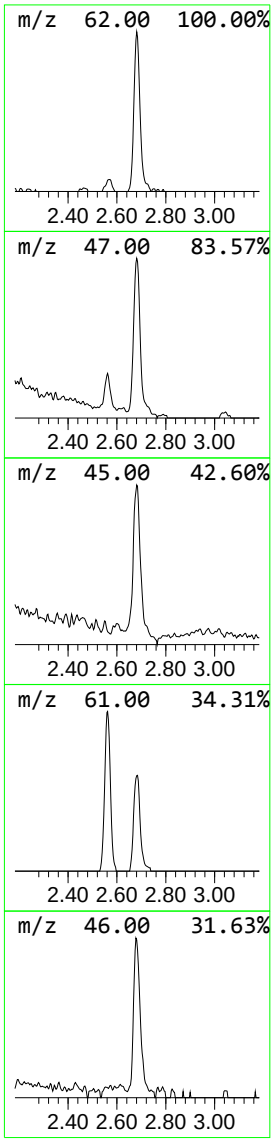
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Dimethyl sulfide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.681	0.78 ug/L	63637	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	95
2	Dimethyl sulfide	62	C2H6S	000075-18-3	94
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Dimethyl sulfide	62	C2H6S	000075-18-3	91
5	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90





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Instrument :
MSVOA_U
ClientSampleId :
DBWN4

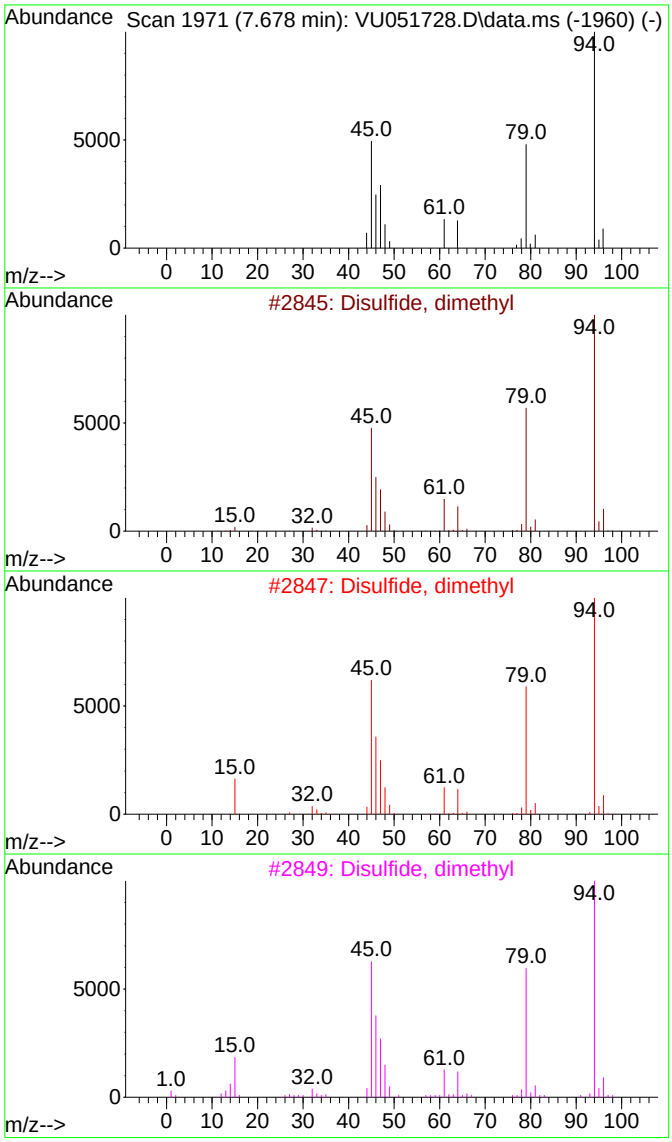
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

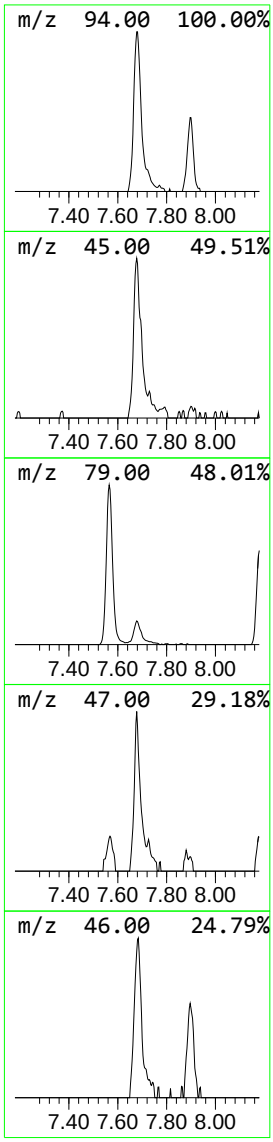
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Disulfide, dimethyl Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.678	0.59 ug/L	47611	1,4-Difluorobenzene	6.247

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	97
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	94
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91





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Instrument :
MSVOA_U
ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102822WMA.M
Quant Title : TRACE VOA SFAM1.0

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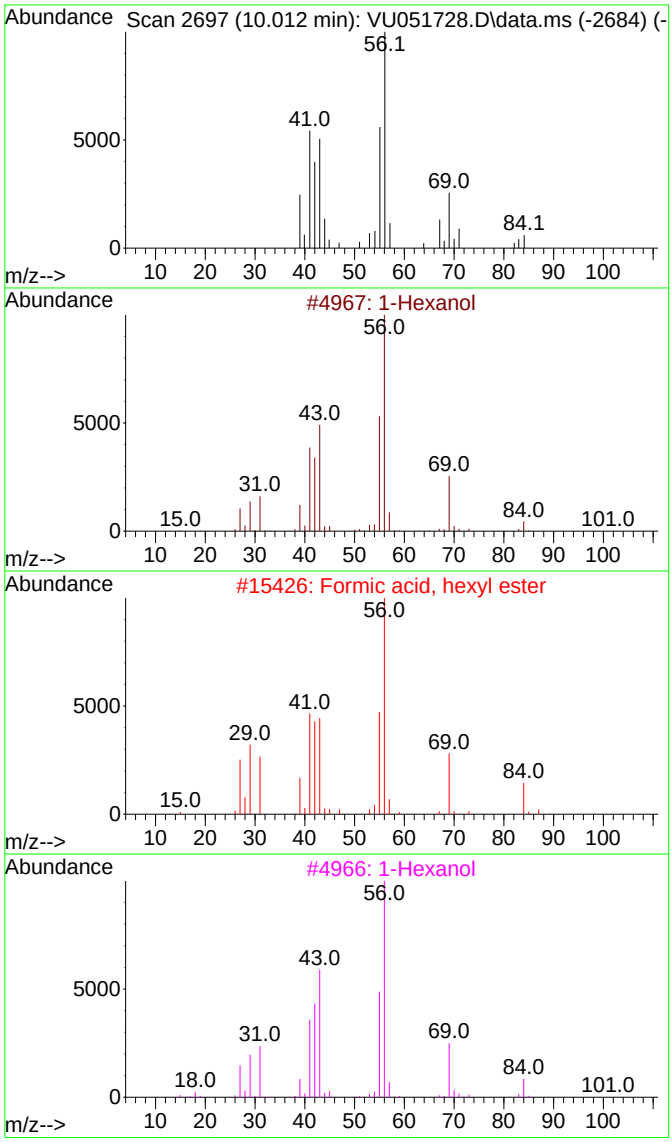
TIC Integration Parameters: LSCINT.P

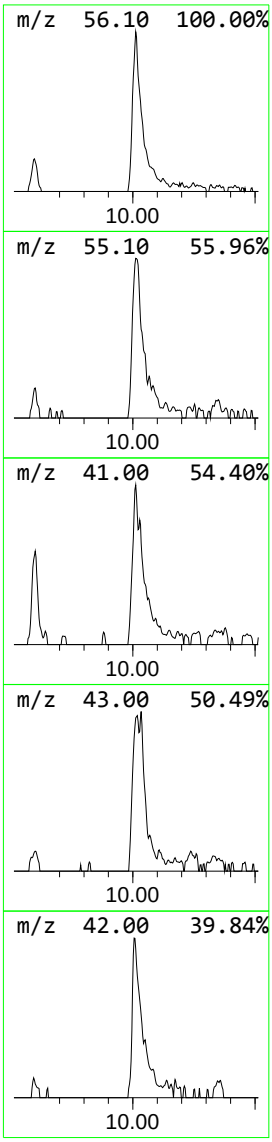
****

Peak Number 5 1-Hexanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.012	0.62 ug/L	69426	Chlorobenzene-d5	9.417

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol	102	C6H14O	000111-27-3	72
2	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64
3	1-Hexanol	102	C6H14O	000111-27-3	64
4	Formic acid, hexyl ester	130	C7H14O2	000629-33-4	64
5	1-Hexanol	102	C6H14O	000111-27-3	64





Tentatively Identified Compound (LSC) summary

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Quant Title : TRACE VOA SFAM1.0

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Methanethiol	1.784	5.7	ug/L	465424	1	6.247	405650	5.0
Dimethyl sulfide	2.681	0.8	ug/L	63637	1	6.247	405650	5.0
Disulfide, dime...	7.678	0.6	ug/L	47611	1	6.247	405650	5.0
1-Hexanol	10.012	0.6	ug/L	69426	2	9.417	556326	5.0