

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU011325\
 Data File : VU062718.D
 Acq On : 13 Jan 2025 15:34
 Operator : MD/SY
 Sample : Q1059-02
 Misc : 25mL/MSVOA_U/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH8Z1

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\SFAMUTR010225WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU062718.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	86	95	110	rVB2	43283	57206	6.91%	1.565%
2	1.782	144	153	166	rBV	44658	62086	7.50%	1.699%
3	1.904	183	191	201	rBV	23334	31267	3.78%	0.856%
4	2.563	383	396	409	rBV4	84367	165917	20.04%	4.540%
5	2.673	421	430	441	rVB2	14979	26129	3.16%	0.715%
6	2.943	494	514	537	rBV4	7872	24090	2.91%	0.659%
7	3.856	784	798	820	rBB	22499	53802	6.50%	1.472%
8	4.650	1025	1045	1080	rBV3	288507	827927	100.00%	22.655%
9	5.049	1155	1169	1193	rBV2	57766	129503	15.64%	3.544%
10	5.711	1357	1375	1400	rBV3	100001	269028	32.49%	7.361%
11	6.238	1527	1539	1562	rBV	102225	200359	24.20%	5.482%
12	6.531	1619	1630	1649	rBV2	84660	163771	19.78%	4.481%
13	6.679	1664	1676	1696	rBV2	61577	120963	14.61%	3.310%
14	7.557	1939	1949	1968	rBV2	28664	51285	6.19%	1.403%
15	7.669	1973	1984	2012	rBV3	26519	79200	9.57%	2.167%
16	7.888	2041	2052	2069	rBV	128956	227192	27.44%	6.217%
17	8.174	2131	2141	2159	rBV	18294	31993	3.86%	0.875%
18	8.624	2269	2281	2309	rBV2	134671	267888	32.36%	7.330%
19	8.782	2321	2330	2341	rBV5	9063	15780	1.91%	0.432%
20	9.409	2514	2525	2547	rBV	146388	245801	29.69%	6.726%
21	10.746	2930	2941	2956	rBV	53196	84992	10.27%	2.326%
22	11.354	3119	3130	3149	rBV2	31161	57968	7.00%	1.586%
23	11.804	3259	3270	3289	rBV	146883	242244	29.26%	6.629%
24	12.184	3374	3388	3409	rBV	130019	218149	26.35%	5.969%

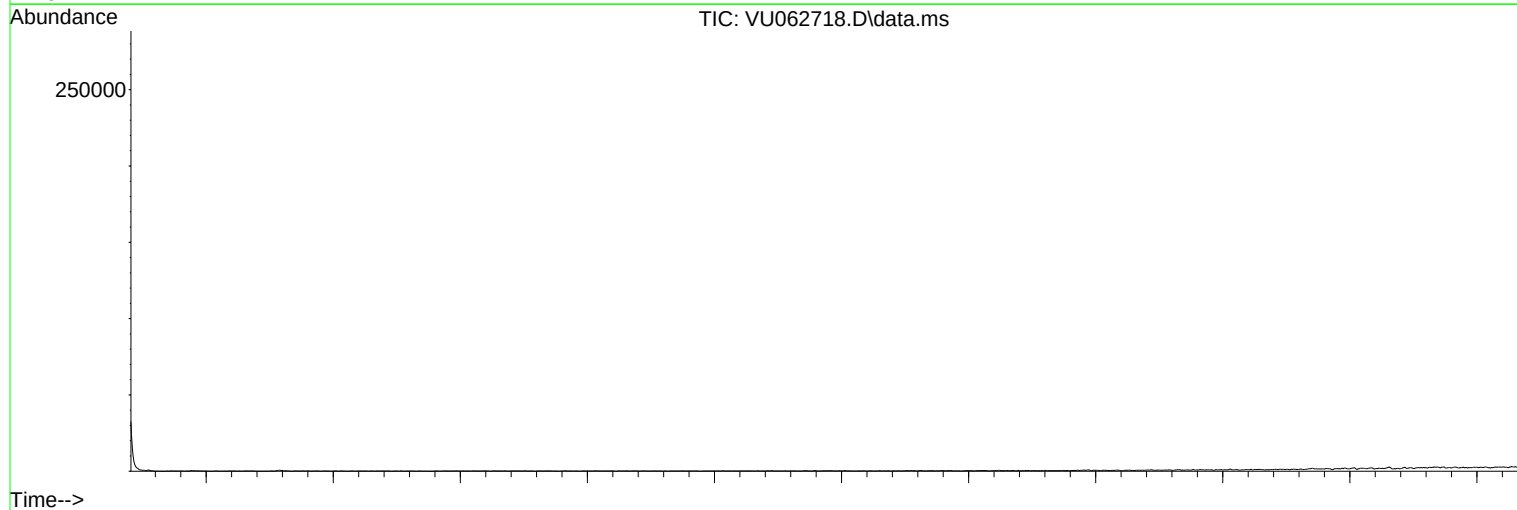
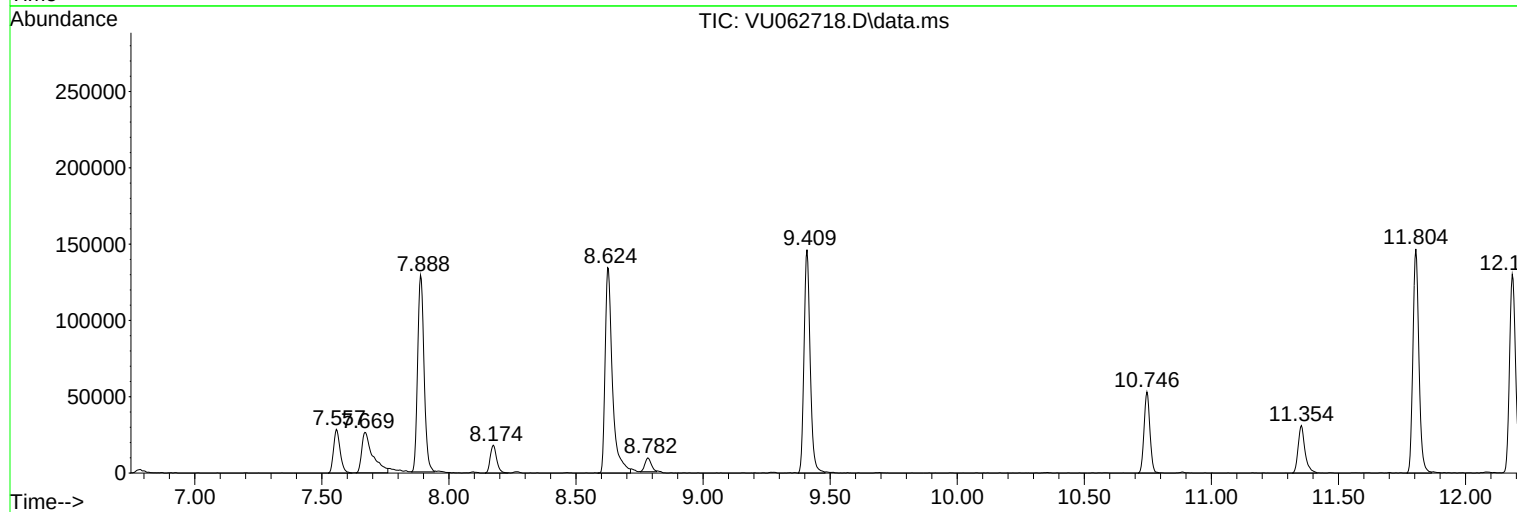
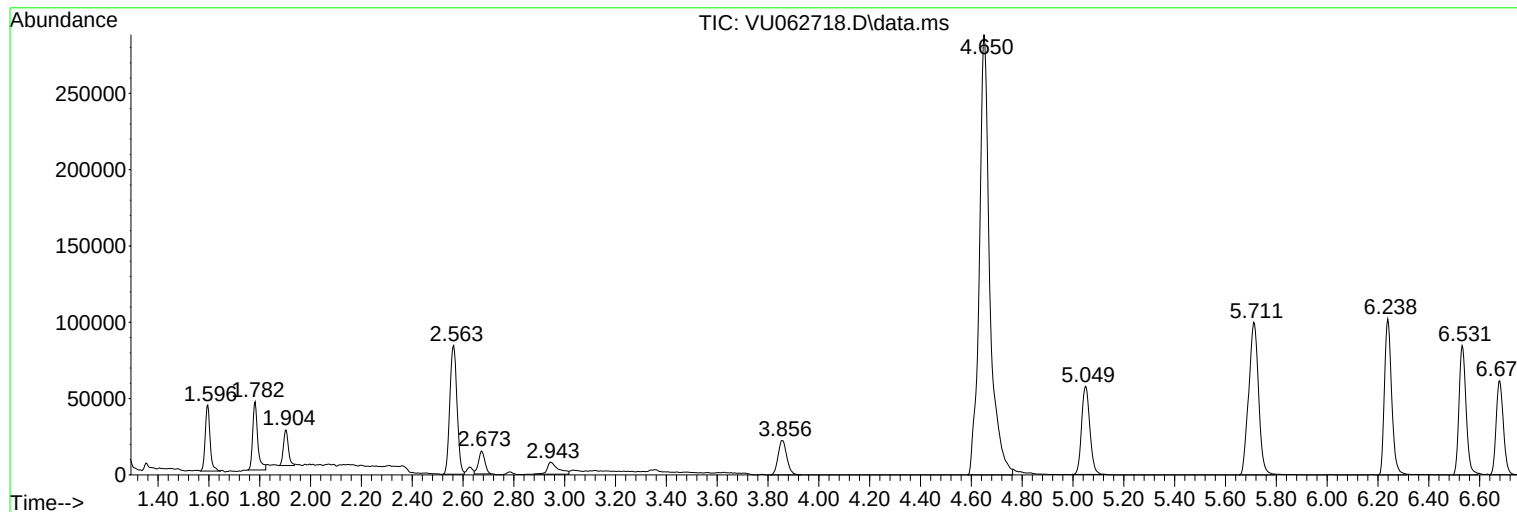
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

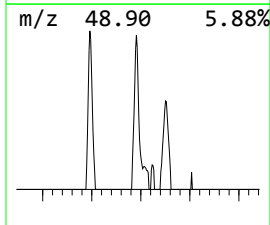
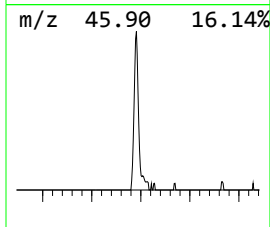
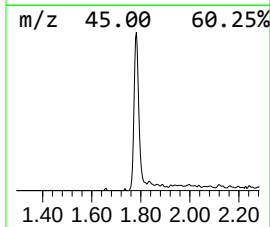
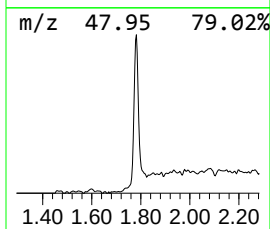
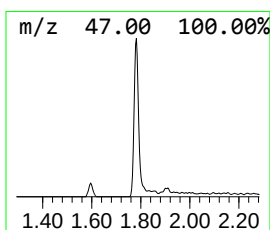
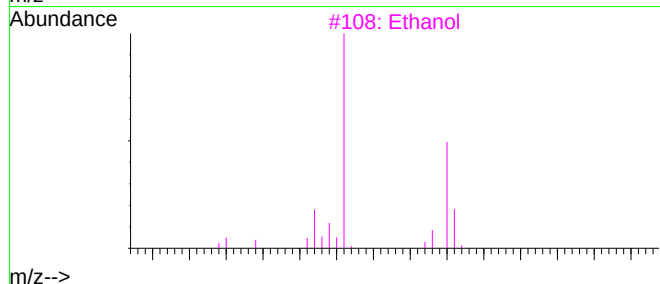
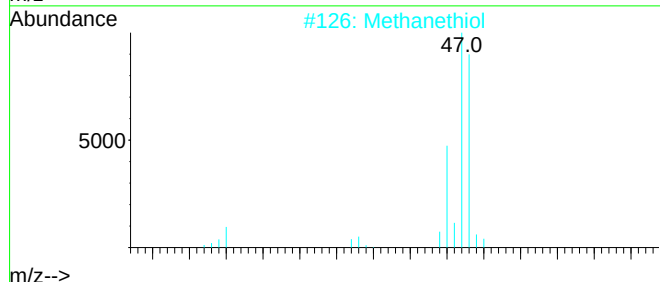
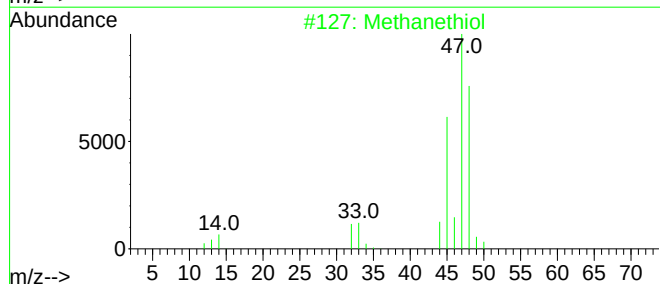
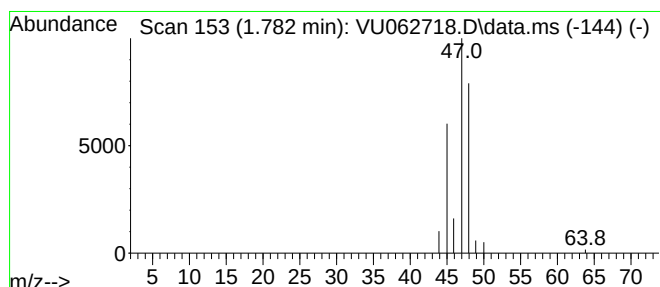
TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 1 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.782	1.55 ug/L	62086	1,4-Difluorobenzene	6.238

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methanethiol	48	CH4S	000074-93-1	91
2	Methanethiol	48	CH4S	000074-93-1	90
3	Ethanol	46	C2H6O	000064-17-5	4
4	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4
5	Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	4



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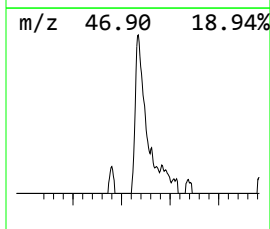
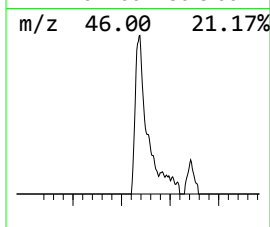
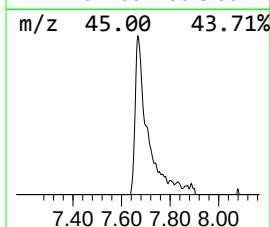
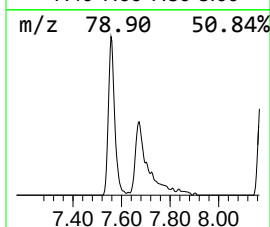
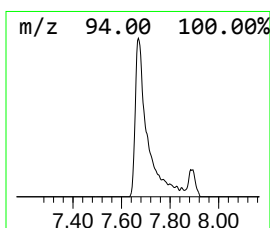
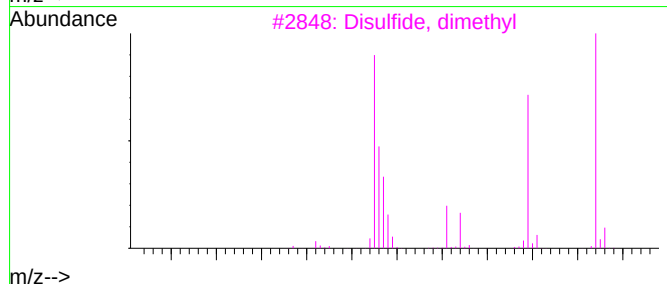
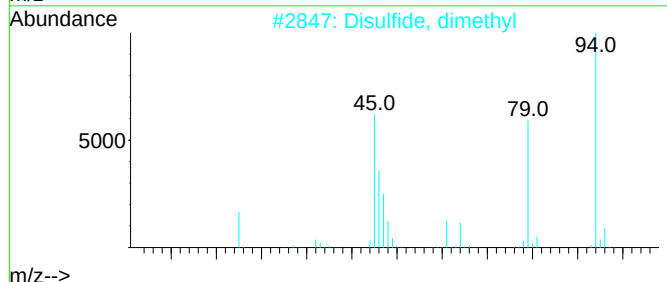
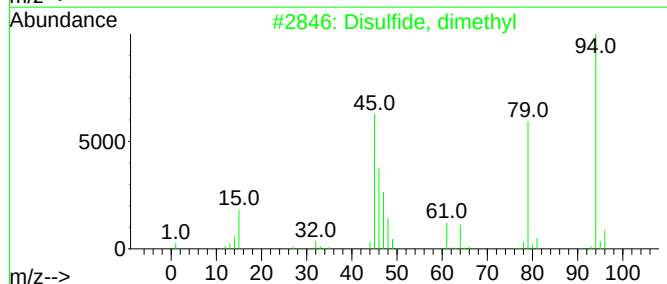
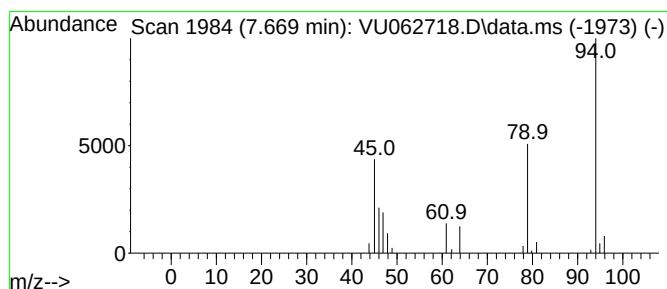
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 3 Disulfide, dimethyl Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.	
7.669	1.98 ug/L	79200	1,4-Difluorobenzene	6.238	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
2	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
3	Disulfide, dimethyl	94	C2H6S2	000624-92-0	91
4	Disulfide, dimethyl	94	C2H6S2	000624-92-0	90
5	Disulfide, dimethyl	94	C2H6S2	000624-92-0	86



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ALS Vial : 18 Sample Multiplier: 1

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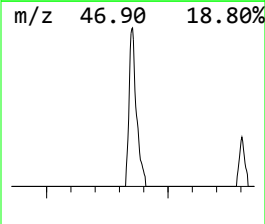
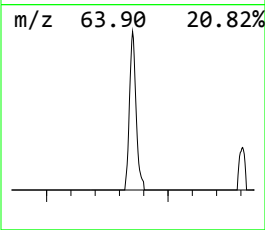
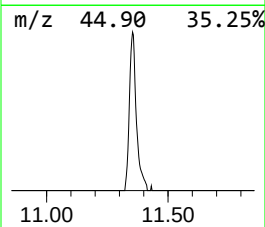
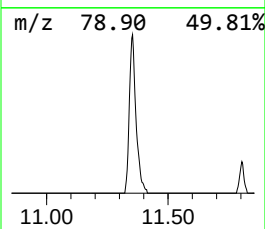
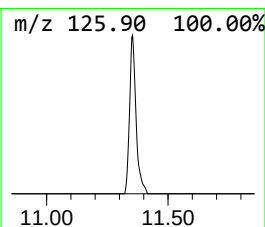
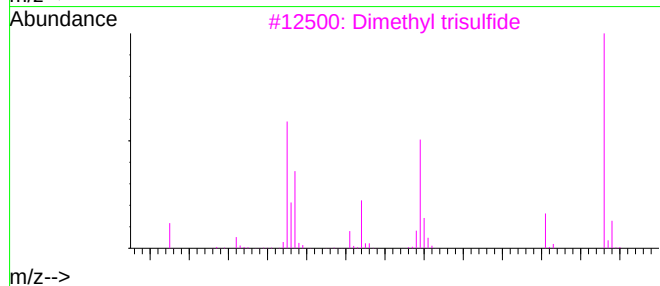
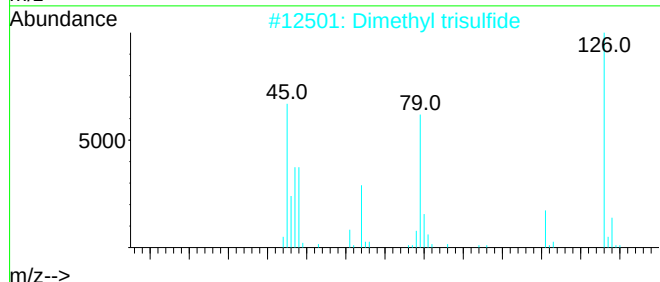
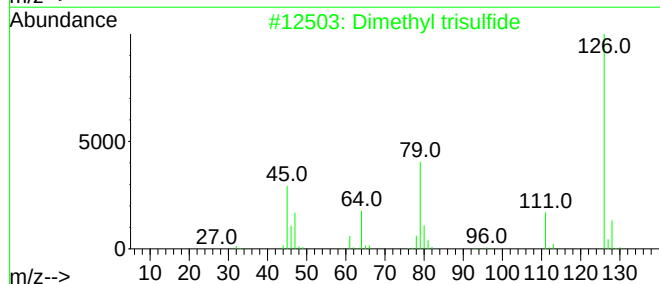
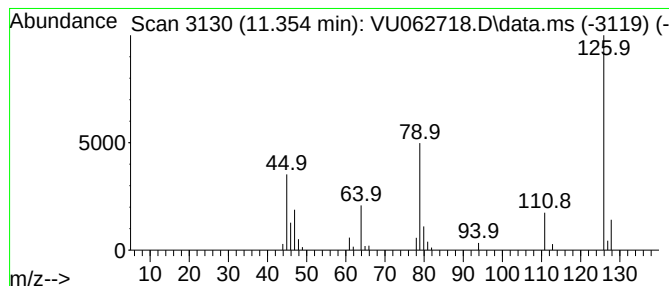
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR010225WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P

Peak Number 4 Dimethyl trisulfide Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.354	1.20 ug/L	57968	1,4-Dichlorobenzene-d4		11.804	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Dimethyl trisulfide		126	C2H6S3	003658-80-8	96
2	Dimethyl trisulfide		126	C2H6S3	003658-80-8	94
3	Dimethyl trisulfide		126	C2H6S3	003658-80-8	94
4	Dimethyl trisulfide		126	C2H6S3	003658-80-8	72
5	Dimethyl trisulfide		126	C2H6S3	003658-80-8	43



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.782	1.6	ug/L	62086	1	6.238	200359	5.0
Disulfide, dime...	7.669	2.0	ug/L	79200	1	6.238	200359	5.0
Dimethyl trisul...	11.354	1.2	ug/L	57968	3	11.804	242244	5.0