LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028919.D
Acq On : 12 Nov 2022 09:32
Operator : SY/MD
Sample : N5602-17
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG9

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_V\Method\SFAMVTR111122WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VV028919.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	14	20	30	rBV2	65220	70254	7.41%	0.734%
2	1.207	48	52	57	rVB	40647	32467	3.42%	0.339%
3	1.297	71	80	91	rBV2	144155	185465	19.55%	1.938%
4	1.410	106	115	127	rBV	837639	948711	100.00%	9.913%
5	1.561	155	162	174	rVV	112847	130742	13.78%	1.366%
6	1.632	175	184	199	rVB2	39884	77275	8.15%	0.807%
7	1.796	229	235	246	rBV4	13284	25103	2.65%	0.262%
8	2.098	320	329	346	rVB	199263	292908	30.87%	3.060%
9	2.201	353	361	375	rBV	94610	141425	14.91%	1.478%
10	3.969	887	911	925	rBV2	38121	166321	17.53%	1.738%
11	4.336	1010	1025	1047	rBV2	138466	335929	35.41%	3.510%
12	5.034	1226	1242	1267	rBV2	368848	843412	88.90%	8.812%
13	5.185	1280	1289	1299	rBV6	9383	18229	1.92%	0.190%
14	5.583	1399	1413	1432	rBV	243615	481239	50.73%	5.028%
15	5.863	1492	1500	1514	rBV	8821	18858	1.99%	0.197%
16	6.040	1542	1555	1576	rBV	167565	354954	37.41%	3.709%
17	6.474	1681	1690	1693	rBV3	6007	10092	1.06%	0.105%
18	6.616	1727	1734	1752	rVB3	8608	18811	1.98%	0.197%
19	6.992	1837	1851	1865	rBV	67970	123574	13.03%	1.291%
20	7.082	1875	1879	1893	rBV	20052	29845	3.15%	0.312%
21	7.175	1899	1908	1924	rVB	31484	59859	6.31%	0.625%
22	7.268	1928	1937	1941	rVV4	7206	12428	1.31%	0.130%
23	7.317	1941	1952	1967	rVV	481999	848593	89.45%	8.867%
24	7.387	1969	1974	1987	rVB4	23040	41622	4.39%	0.435%
25	7.632	2040	2050	2063	rBV2	35389	62168	6.55%	0.650%
26	8.117	2184	2201	2232	rBV3	328573	826644	87.13%	8.637%
27	8.853	2417	2430	2458	rBV	450594	776164	81.81%	8.110%
28	9.140	2510	2519	2534	rVB5	13949	24843	2.62%	0.260%
29	9.548	2636	2646	2662	rVB	7109	11539	1.22%	0.121%
30	10.217	2840	2854	2870	rBV	151548	251169	26.47%	2.624%
31	10.773	3020	3027	3038	rVB9	5119	9567	1.01%	0.100%
32	10.911	3061	3070	3080	rBV3	9194	15278	1.61%	0.160%
33	11.242	3161	3173	3194	rBV	500177	792573	83.54%	8.281%
34	11.332	3194	3201	3212	rVB4	8556	16703	1.76%	0.175%
35	11.529	3250	3262	3271	rBV9	10703	23332	2.46%	0.244%
36	11.619	3277	3290	3313	rVB	459177	760869	80.20%	7.950%

LSC Area Percent Report

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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_V\Method\SFAMVTR111122WMA.M
Title : TRACE VOA SFAM1.0

37	12.059	3420	3427	3435	rVB	7847	13474	1.42%	0.141%
38	12.242	3473	3484	3492	rBV	5776	12572	1.33%	0.131%
39	12.458	3544	3551	3561	rVB3	11514	18617	1.96%	0.195%
40	12.869	3672	3679	3693	rVB5	15444	27660	2.92%	0.289%
41	13.053	3727	3736	3753	rVB5	8991	27628	2.91%	0.289%
42	13.156	3758	3768	3774	rBV5	7272	11825	1.25%	0.124%
43	13.210	3777	3785	3791	rVB6	7310	9847	1.04%	0.103%
44	13.258	3792	3800	3806	rBV5	12779	19464	2.05%	0.203%
45	13.467	3854	3865	3867	rBV9	8893	13310	1.40%	0.139%
46	13.493	3867	3873	3883	rVV	20303	37955	4.00%	0.397%
47	13.532	3883	3885	3897	rVB3	7978	11654	1.23%	0.122%
48	13.599	3897	3906	3910	rBV5	13316	22741	2.40%	0.238%
49	13.628	3911	3915	3923	rVV2	14211	21435	2.26%	0.224%
50	13.686	3924	3933	3948	rVB2	18765	40548	4.27%	0.424%
51	13.914	3991	4004	4019	rVB10	16416	39104	4.12%	0.409%
52	13.995	4020	4029	4037	rBV5	21884	37077	3.91%	0.387%
53	14.098	4049	4061	4069	rBV5	10909	27155	2.86%	0.284%
54	14.139	4069	4074	4080	rVB7	8951	12506	1.32%	0.131%
55	14.207	4087	4095	4098	rBV8	9643	14568	1.54%	0.152%
56	14.274	4107	4116	4128	rBV5	32670	71743	7.56%	0.750%
57	14.429	4155	4164	4177	rVB9	13904	29064	3.06%	0.304%
58	14.564	4198	4206	4211	rBV9	6332	10648	1.12%	0.111%
59	14.606	4211	4219	4221	rBV5	11352	14366	1.51%	0.150%
60	14.731	4250	4258	4264	rBV3	12934	21852	2.30%	0.228%
61	14.808	4276	4282	4291	rVB5	11960	19591	2.07%	0.205%
62	15.323	4437	4442	4452	rVB7	9872	14721	1.55%	0.154%
63	15.802	4586	4591	4597	rBV5	7644	10892	1.15%	0.114%
64	15.860	4598	4609	4610	rBV7	15619	26791	2.82%	0.280%
65	16.168	4697	4705	4720	rBV2	56142	92892	9.79%	0.971%

Sum of corrected areas: 9570665

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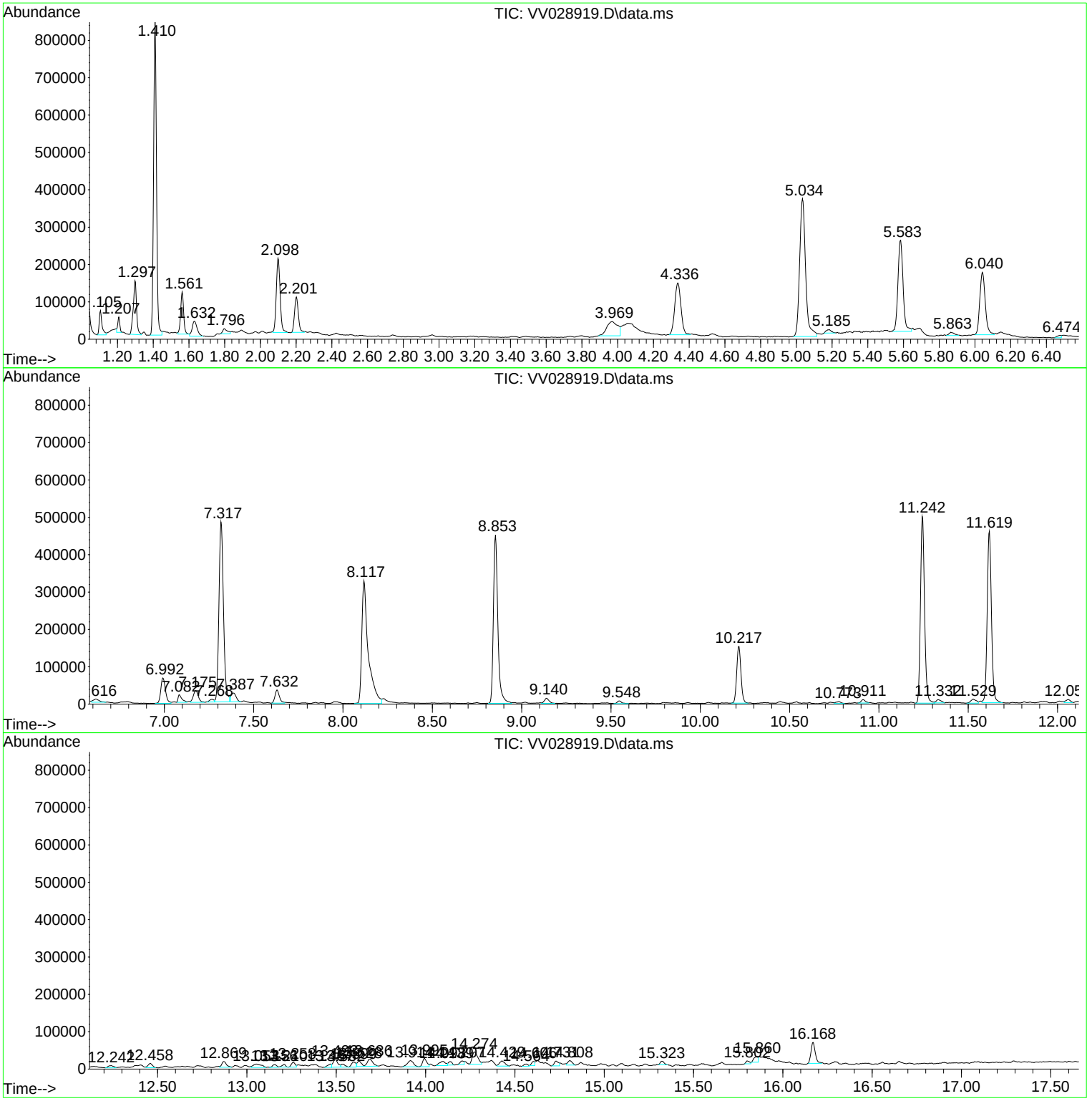
Instrument :
MSVOA_V
ClientSampleId :
C0AG9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
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MSVOA_V
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C0AG9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

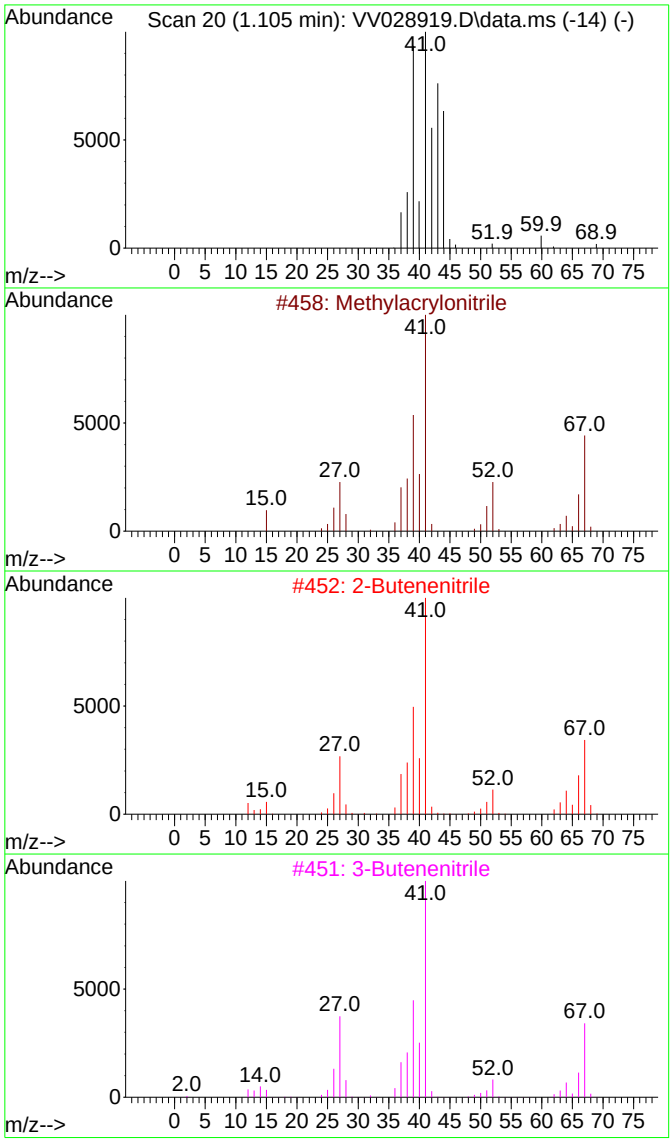
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

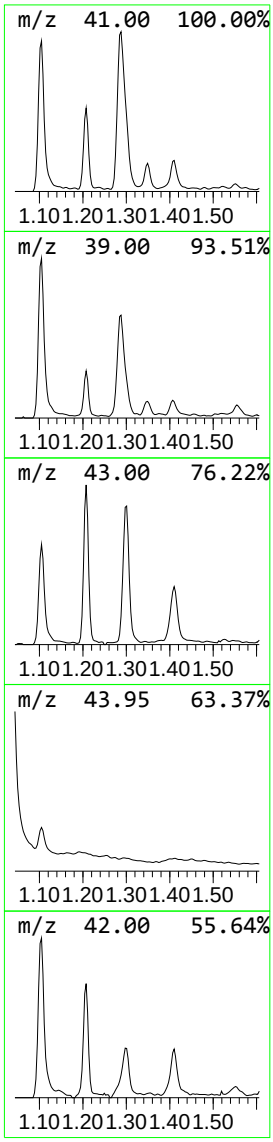
****

Peak Number 1 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.105	0.73 ug/L	70254	1,4-Difluorobenzene	5.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methylacrylonitrile	67	C4H5N	000126-98-7	10
2	2-Butenenitrile	67	C4H5N	004786-20-3	9
3	3-Butenenitrile	67	C4H5N	000109-75-1	9
4	Chloro(prop-2-yn-1-yloxy)methanone	118	C4H3ClO2	035718-08-2	9
5	Propene	42	C3H6	000115-07-1	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV111122\
Data File : VV028919.D
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Operator : SY/MD
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ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG9

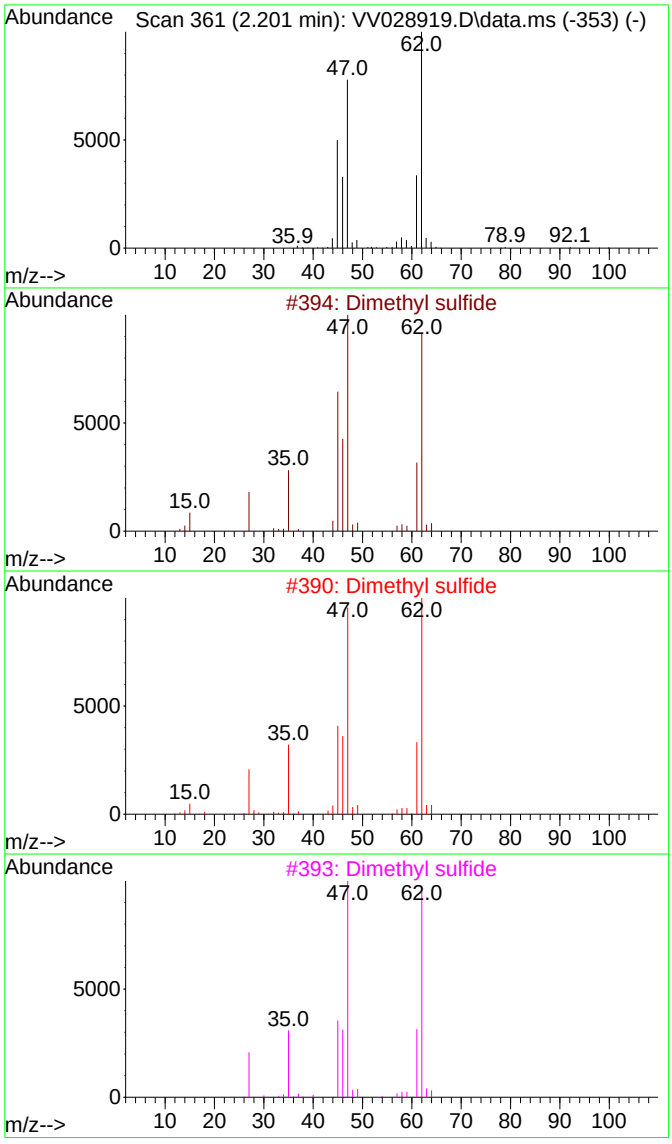
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

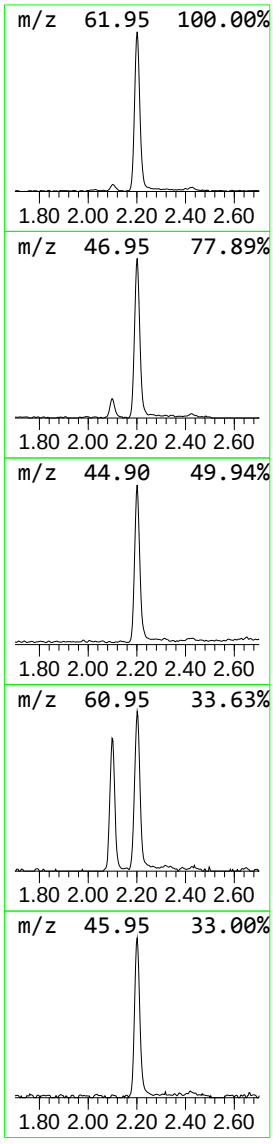
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Dimethyl sulfide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.201	1.47 ug/L	141425	1,4-Difluorobenzene	5.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dimethyl sulfide	62	C2H6S	000075-18-3	94
2	Dimethyl sulfide	62	C2H6S	000075-18-3	91
3	Dimethyl sulfide	62	C2H6S	000075-18-3	91
4	Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	83
5	Ethanethiol	62	C2H6S	000075-08-1	78





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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG9

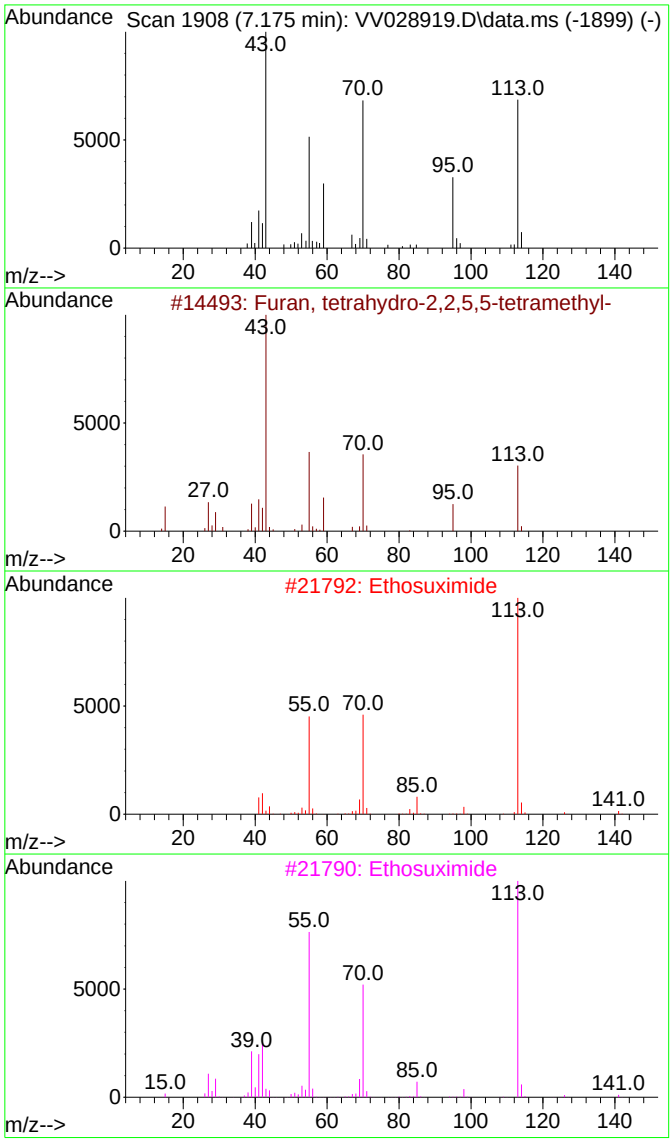
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

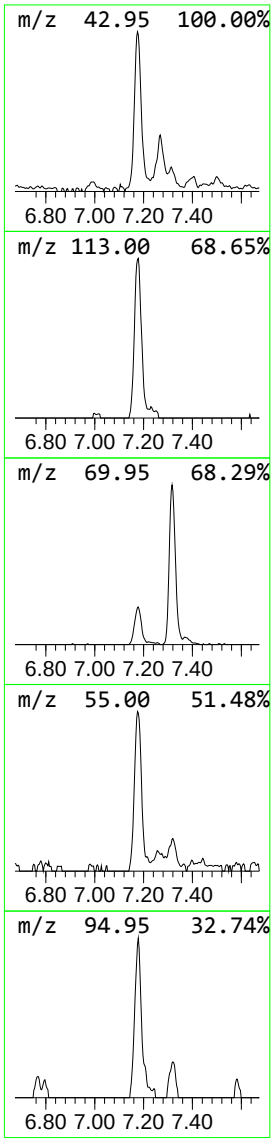
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Furan, tetrahydro-2,2,5,5-t... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.175	0.62 ug/L	59859	1,4-Difluorobenzene	5.583

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, tetrahydro-2,2,5,5-tetram...	128	C8H16O	015045-43-9	83
2	Ethosuximide	141	C7H11NO2	000077-67-8	47
3	Ethosuximide	141	C7H11NO2	000077-67-8	47
4	1,3,5-Triazine-2,4(1H,3H)-dione	113	C3H3N3O2	000071-33-0	43
5	Furan, tetrahydro-2,2,4,4-tetram...	128	C8H16O	003358-28-9	42





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ALS Vial : 53 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AG9

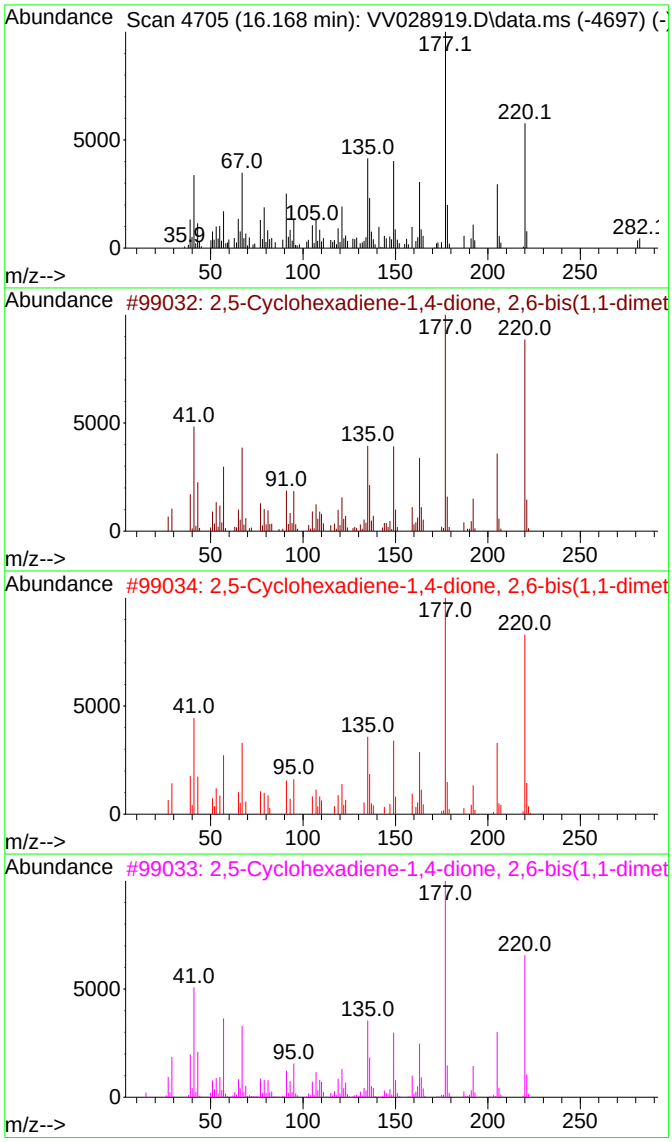
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR111122WMA.M
Quant Title : TRACE VOA SFAM1.0

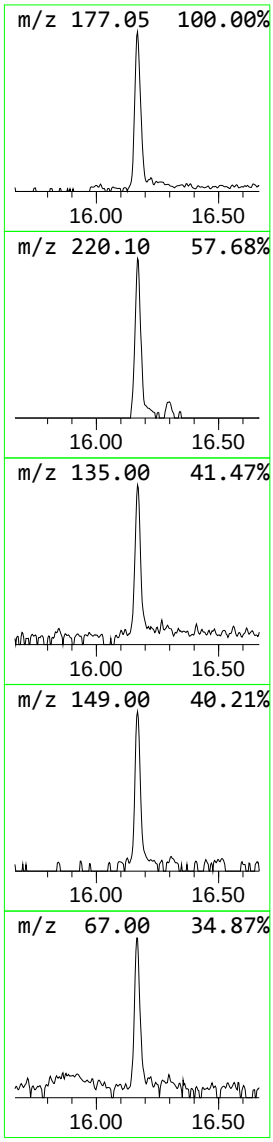
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.168	0.59 ug/L	92892	1,4-Dichlorobenzene-d4	11.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	98
2	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
3	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
4	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	96
5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	94





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
unknown-01	1.105	0.7	ug/L	70254	1	5.583	481239	5.0
Dimethyl sulfide	2.201	1.5	ug/L	141425	1	5.583	481239	5.0
Furan, tetrahyd...	7.175	0.6	ug/L	59859	1	5.583	481239	5.0
2,5-Cyclohexadi...	16.168	0.6	ug/L	92892	3	11.242	792573	5.0