LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059878.D
Acq On : 08 Jul 2024 13:08
Operator : MD/SY
Sample : VIBLK112
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU059878.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	85	95	106	rBV	65687	82784	15.66%	1.682%
2	1.872	176	181	186	rBV	12866	15357	2.90%	0.312%
3	1.907	186	192	207	rVB	54097	72774	13.76%	1.479%
4	2.560	383	395	410	rVB	95082	156858	29.66%	3.188%
5	3.042	535	545	556	rVB3	4368	8237	1.56%	0.167%
6	3.177	575	587	603	rVB2	3951	9186	1.74%	0.187%
7	4.653	1022	1046	1068	rBV5	24319	94396	17.85%	1.918%
8	5.055	1156	1171	1195	rBV	102922	234176	44.29%	4.759%
9	5.717	1357	1377	1408	rBV3	195265	528778	100.00%	10.746%
10	6.245	1528	1541	1566	rBV	185096	355681	67.26%	7.228%
11	6.534	1621	1631	1643	rVB7	4592	9396	1.78%	0.191%
12	6.685	1662	1678	1700	rBV	132485	259715	49.12%	5.278%
13	7.563	1939	1951	1973	rBV2	40154	74961	14.18%	1.523%
14	7.894	2041	2054	2073	rBV	220861	388958	73.56%	7.905%
15	8.180	2131	2143	2156	rBV2	23608	42084	7.96%	0.855%
16	8.309	2175	2183	2196	rVB5	3602	6487	1.23%	0.132%
17	8.473	2223	2234	2247	rBV8	2726	6121	1.16%	0.124%
18	8.627	2272	2282	2319	rBV	235965	465471	88.03%	9.460%
19	8.910	2358	2370	2377	rBV4	3689	6247	1.18%	0.127%
20	9.412	2513	2526	2546	rBV	260636	448420	84.80%	9.113%
21	10.495	2853	2863	2873	rBV6	4312	6819	1.29%	0.139%
22	10.749	2930	2942	2964	rBV2	114062	187500	35.46%	3.811%
23	11.807	3254	3271	3294	rVB	242162	407996	77.16%	8.292%
24	12.151	3367	3378	3380	rBV2	19936	25489	4.82%	0.518%
25	12.187	3381	3389	3407	rVB	220216	376821	71.26%	7.658%
26	13.344	3741	3749	3758	rBV9	3358	5606	1.06%	0.114%
27	13.408	3758	3769	3780	rBV2	18468	31385	5.94%	0.638%
28	13.614	3818	3833	3840	rBV2	5283	11827	2.24%	0.240%
29	13.669	3843	3850	3861	rVV2	10522	18726	3.54%	0.381%
30	13.730	3862	3869	3879	rVB8	6163	9791	1.85%	0.199%
31	13.894	3911	3920	3928	rVB9	3985	7495	1.42%	0.152%
32	14.016	3950	3958	3967	rVB7	5298	8434	1.59%	0.171%
33	14.106	3976	3986	3994	rBV7	13288	21711	4.11%	0.441%
34	14.158	3994	4002	4014	rVB5	14538	24298	4.60%	0.494%
35	14.347	4051	4061	4069	rBV2	18272	29401	5.56%	0.598%
36	14.508	4093	4111	4123	rBV7	11384	29680	5.61%	0.603%

LSC Area Percent Report

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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

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\SFAMUTR061724WMA.M
Title : TRACE VOA SFAM1.0

37	14.572	4123	4131	4138	rBV9	10364	16292	3.08%	0.331%
38	14.646	4151	4154	4164	rVB7	5320	6076	1.15%	0.123%
39	14.797	4194	4201	4217	rVB7	8824	22451	4.25%	0.456%
40	14.900	4223	4233	4243	rBV7	11667	26695	5.05%	0.543%
41	15.026	4266	4272	4275	rBV4	7614	8757	1.66%	0.178%
42	15.129	4289	4304	4310	rBV9	11705	26089	4.93%	0.530%
43	15.232	4328	4336	4342	rBV9	4848	6804	1.29%	0.138%
44	15.351	4354	4373	4379	rBV6	27893	71776	13.57%	1.459%
45	15.396	4380	4387	4398	rVB7	30114	59622	11.28%	1.212%
46	15.518	4418	4425	4431	rBV5	11842	19123	3.62%	0.389%
47	15.563	4431	4439	4450	rVB7	30973	53304	10.08%	1.083%
48	15.688	4468	4478	4489	rBV7	21987	52753	9.98%	1.072%
49	15.820	4512	4519	4530	rVB7	6230	11110	2.10%	0.226%
50	16.003	4568	4576	4585	rVB4	19256	32451	6.14%	0.659%
51	16.627	4761	4770	4780	rBV5	18289	32780	6.20%	0.666%
52	17.219	4950	4954	4957	rBV6	5024	5442	1.03%	0.111%

Sum of corrected areas: 4920591

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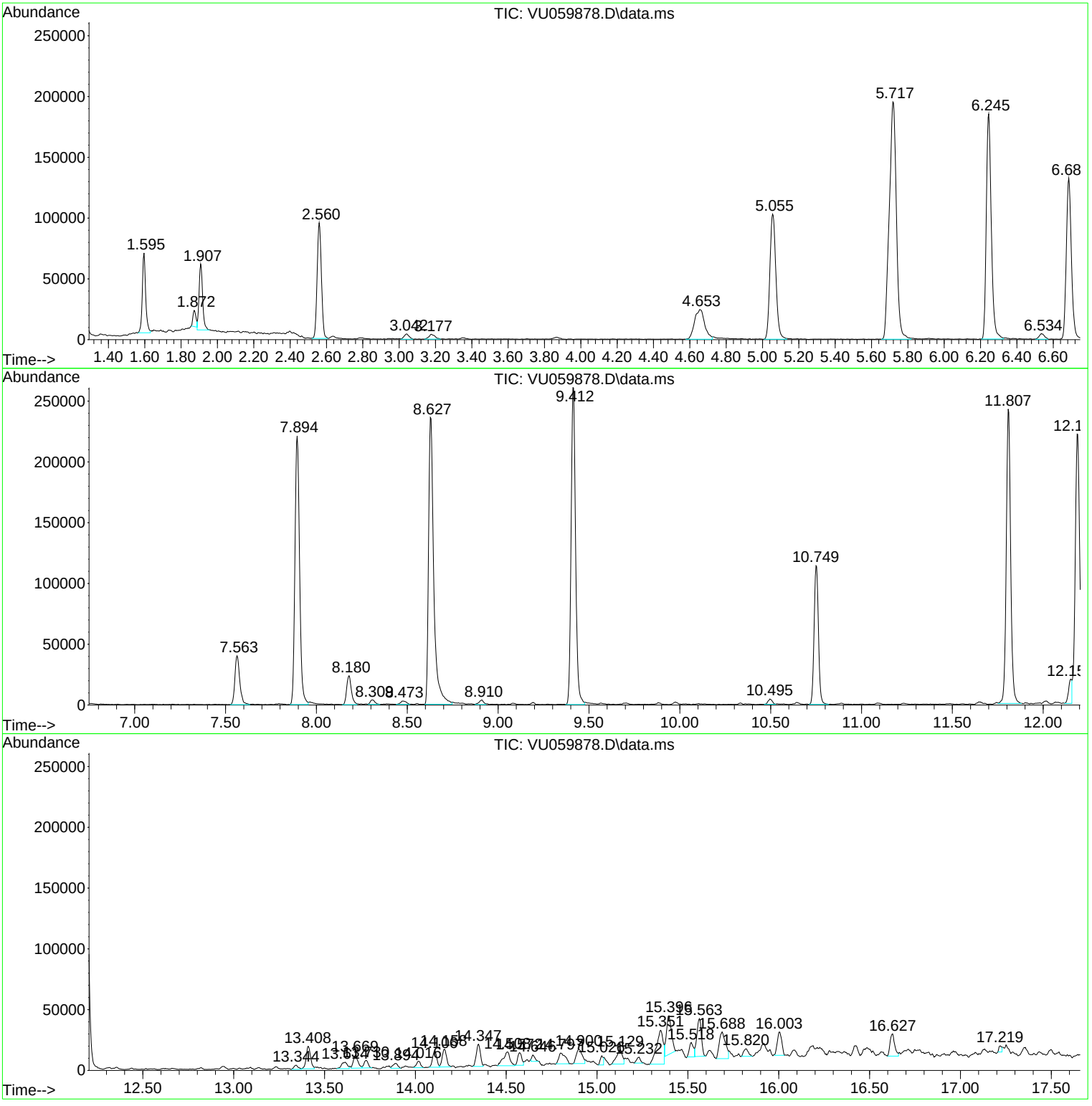
Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070824\
Data File : VU059878.D
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MSVOA_U
ClientSampleId :
VIBLK113

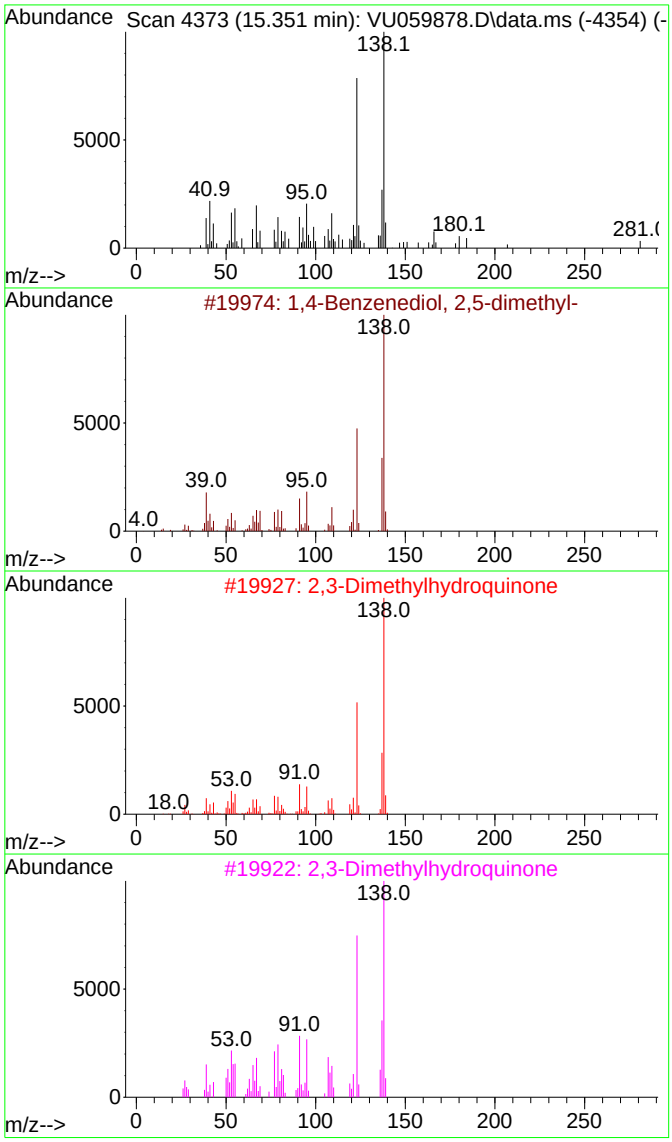
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

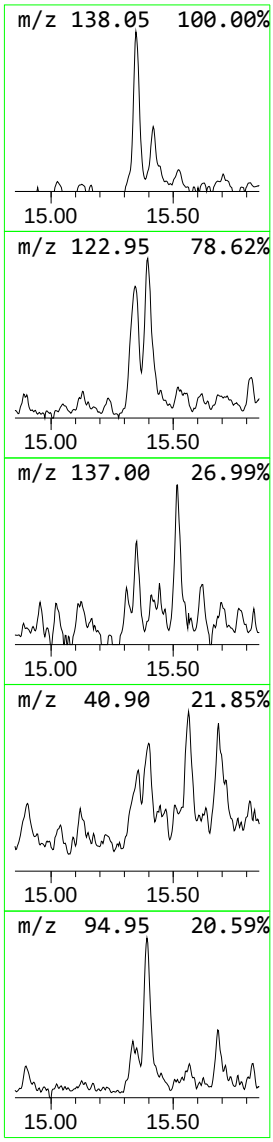
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 1,4-Benzenediol, 2,5-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.351	0.88 ug/L	71776	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,4-Benzenediol, 2,5-dimethyl-	138	C8H10O2	000615-90-7	92
2	2,3-Dimethylhydroquinone	138	C8H10O2	000608-43-5	91
3	2,3-Dimethylhydroquinone	138	C8H10O2	000608-43-5	90
4	2-Ethyl-3-methoxypyrazine	138	C7H10N2O	025680-58-4	80
5	1,4-Benzenediol, 2,6-dimethyl-	138	C8H10O2	000654-42-2	76





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Operator : MD/SY
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

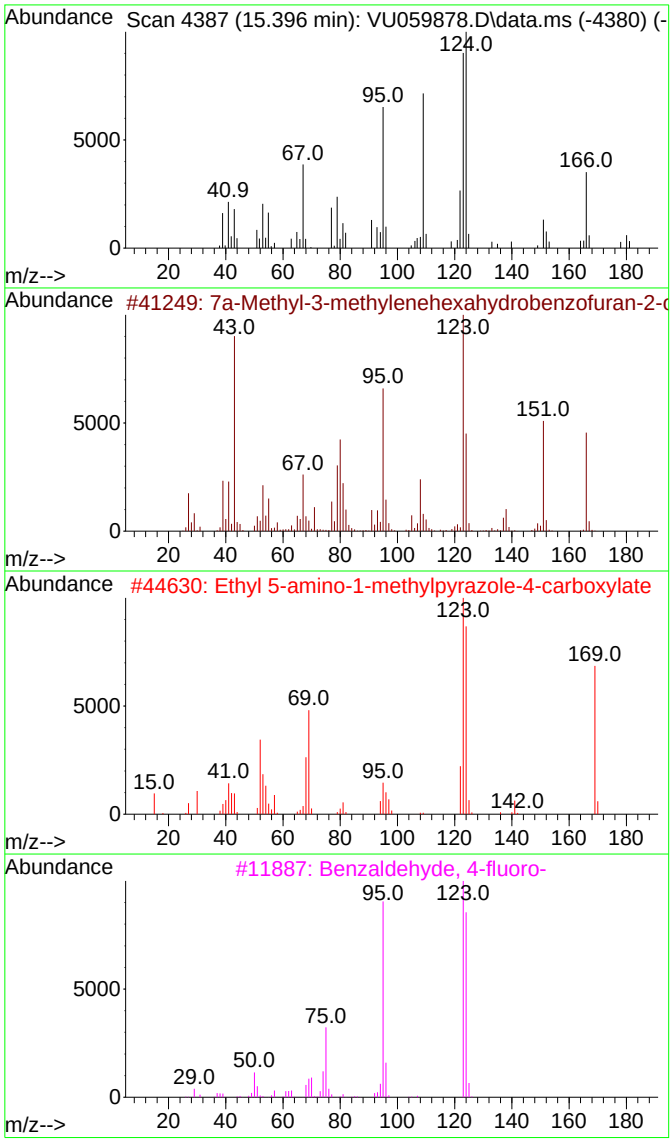
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

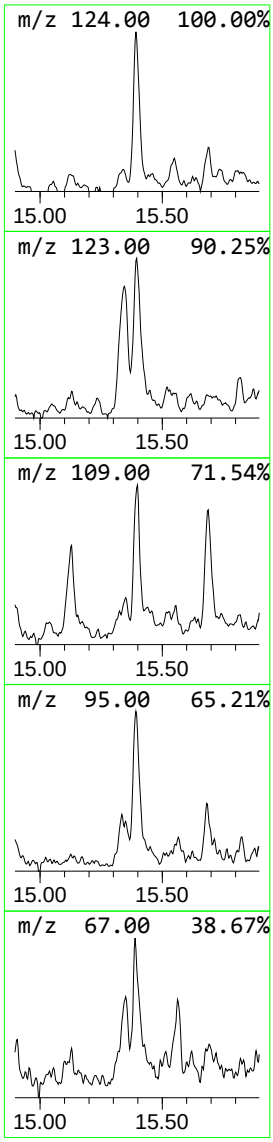
****

Peak Number 3 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.396	0.73 ug/L	59622	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7a-Methyl-3-methylenehexahydrobe...	166	C10H14O2	067498-53-7	49
2	Ethyl 5-amino-1-methylpyrazole-4...	169	C7H11N3O2	031037-02-2	43
3	Benzaldehyde, 4-fluoro-	124	C7H5FO	000459-57-4	43
4	1,6,6-Trimethylbicyclo(3.3.0)oct...	166	C11H18O	1000427-23-1	38
5	2-Cyclopropylthiophene	124	C7H8S	029481-22-9	35





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Operator : MD/SY
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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

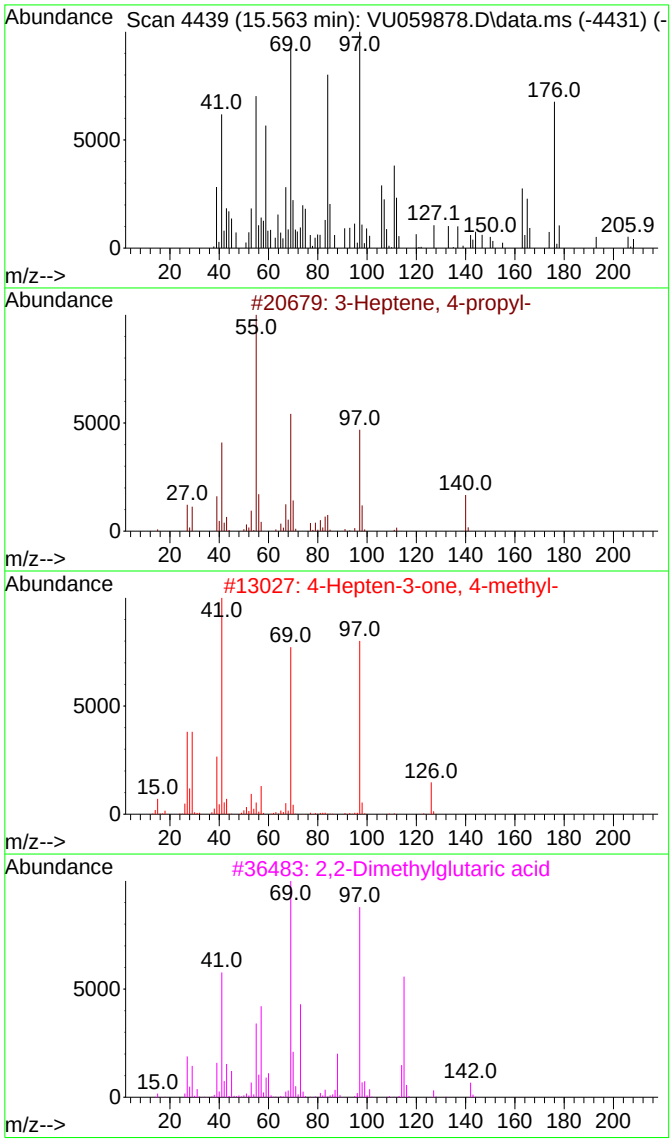
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

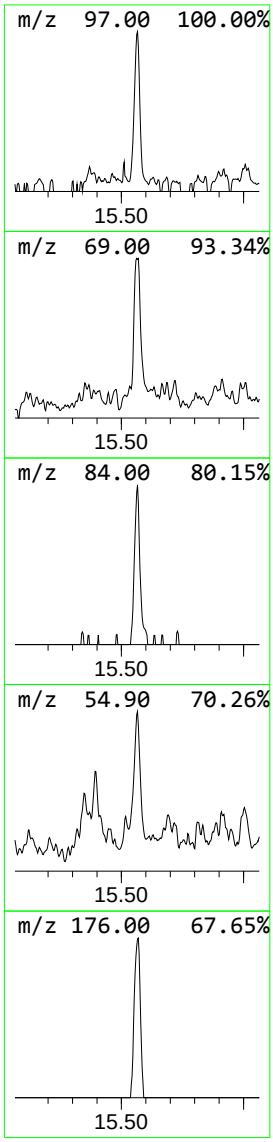
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.563	0.65 ug/L	53304	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 4-propyl-	140	C10H20	004485-13-6	27
2	4-Hepten-3-one, 4-methyl-	126	C8H14O	022319-31-9	22
3	2,2-Dimethylglutaric acid	160	C7H12O4	000681-57-2	22
4	7-Oxabicyclo[4.1.0]heptane, 1-me...	112	C7H12O	001713-33-3	11
5	3,5-Hexadien-2-ol, 2-methyl-	112	C7H12O	000926-38-5	11





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Operator : MD/SY
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ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VIBLK113

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

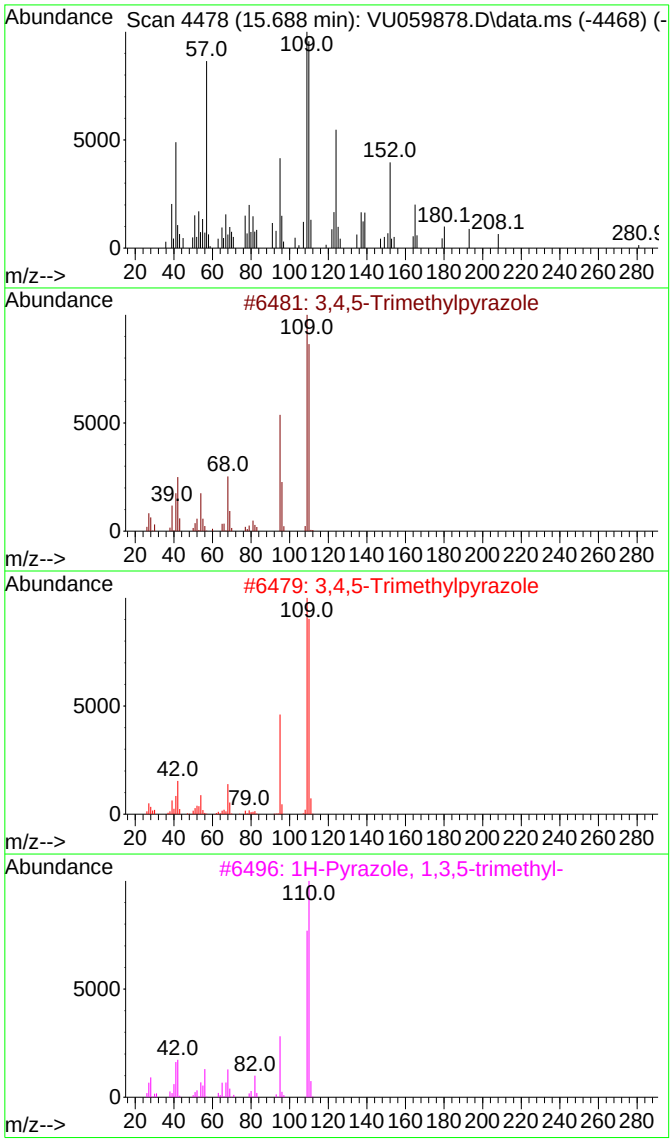
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

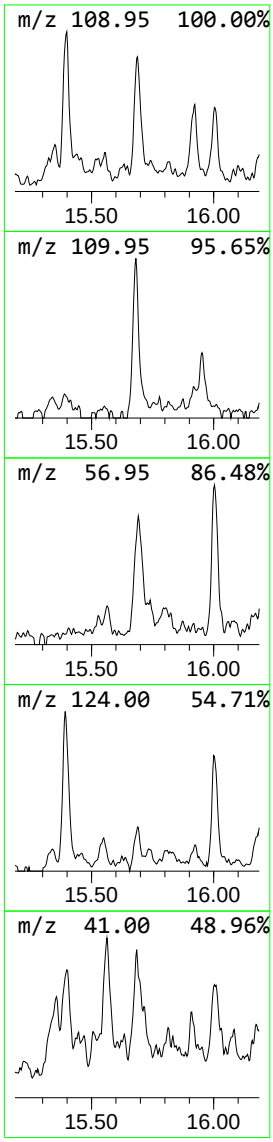
****

Peak Number 5 unknown-02 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.688	0.65 ug/L	52753	1,4-Dichlorobenzene-d4	11.807

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	49
2	3,4,5-Trimethylpyrazole	110	C6H10N2	005519-42-6	49
3	1H-Pyrazole, 1,3,5-trimethyl-	110	C6H10N2	001072-91-9	49
4	1-Methoxybicyclo[2,2,2]oct-5-en-...	180	C11H16O2	1000132-14-1	46
5	3-Heptyne, 2,2-dimethyl-	124	C9H16	029022-29-5	42





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
1,4-Benzenediol...	15.351	0.9	ug/L	71776	3	11.807	407996	5.0
unknown-01	15.396	0.7	ug/L	59622	3	11.807	407996	5.0
(DEL) Alkane: S...	15.563	0.7	ug/L	53304	3	11.807	407996	5.0
unknown-02	15.688	0.7	ug/L	52753	3	11.807	407996	5.0