LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU080822\
Data File : VU050168.D
Acq On : 09 Aug 2022 05:36
Operator : SY/MD
Sample : N4075-12
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 41 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBUX9

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\SFAMUTR080422WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU050168.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	70	80	94	rBV	33132	40547	5.03%	1.072%
2	1.912	170	178	193	rVB	31172	40746	5.06%	1.077%
3	2.102	221	237	253	rBV2	13988	52561	6.53%	1.390%
4	2.199	263	267	278	rVB3	5659	9020	1.12%	0.238%
5	2.330	293	308	343	rBV	18837	83388	10.35%	2.205%
6	2.565	370	381	394	rVB	51295	81691	10.14%	2.160%
7	3.131	546	557	566	rVB3	4720	9389	1.17%	0.248%
8	3.372	613	632	654	rBV	343269	805373	100.00%	21.292%
9	4.006	820	829	842	rVB4	3550	9064	1.13%	0.240%
10	4.517	977	988	1001	rVB4	5324	12076	1.50%	0.319%
11	4.658	1018	1032	1057	rBV2	53812	166723	20.70%	4.408%
12	5.063	1142	1158	1178	rBV	62055	134007	16.64%	3.543%
13	5.723	1345	1363	1385	rBV2	120694	300227	37.28%	7.937%
14	5.951	1419	1434	1451	rVB2	34151	74134	9.20%	1.960%
15	6.250	1513	1527	1543	rBV	94141	176957	21.97%	4.678%
16	6.694	1652	1665	1681	rBV	79150	152895	18.98%	4.042%
17	7.568	1926	1937	1952	rBV	31229	53364	6.63%	1.411%
18	7.896	2024	2039	2055	rBV	119503	206034	25.58%	5.447%
19	8.182	2113	2128	2140	rBV	18722	32109	3.99%	0.849%
20	8.642	2257	2271	2308	rBV3	187793	457403	56.79%	12.093%
21	9.417	2500	2512	2537	rBV	134687	225314	27.98%	5.957%
22	10.758	2915	2929	2945	rVB	74100	118788	14.75%	3.140%
23	11.812	3242	3257	3274	rBV	113000	178873	22.21%	4.729%
24	12.099	3337	3346	3360	rVB3	17780	27260	3.38%	0.721%
25	12.192	3364	3375	3394	rVV	123563	201924	25.07%	5.338%
26	12.571	3483	3493	3502	rBV	22946	33212	4.12%	0.878%
27	12.973	3609	3618	3628	rVB	10483	14606	1.81%	0.386%
28	13.455	3753	3768	3785	rVB2	47022	76699	9.52%	2.028%
29	16.388	4673	4680	4689	rVB4	5880	8101	1.01%	0.214%

Sum of corrected areas: 3782485

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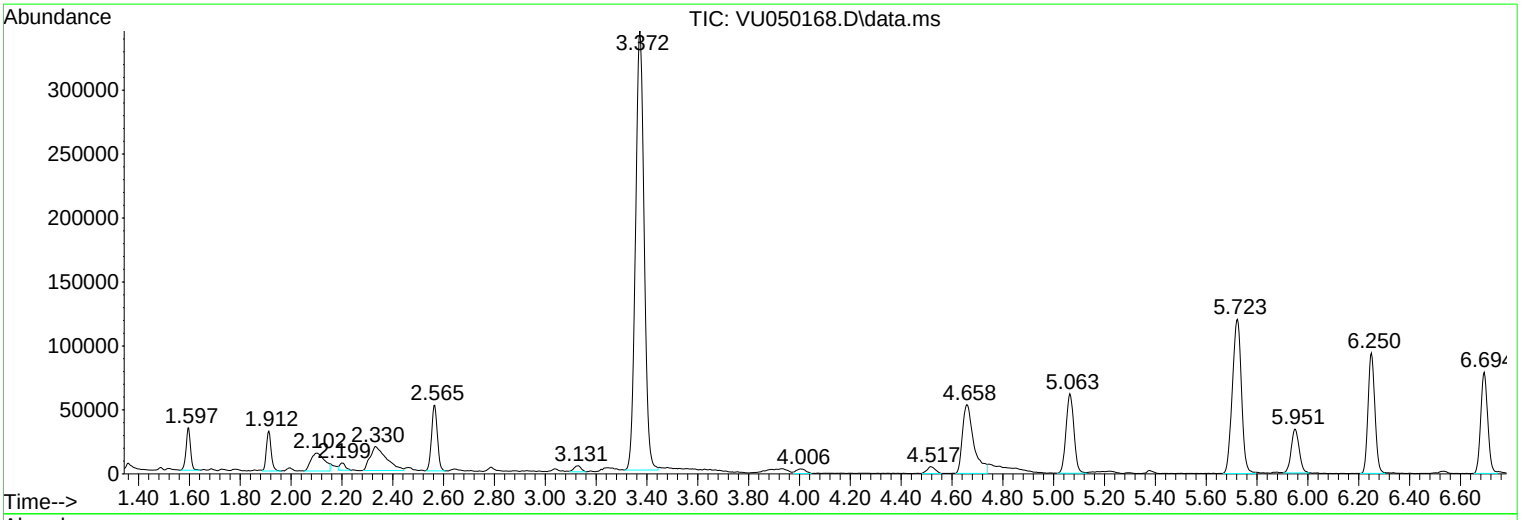
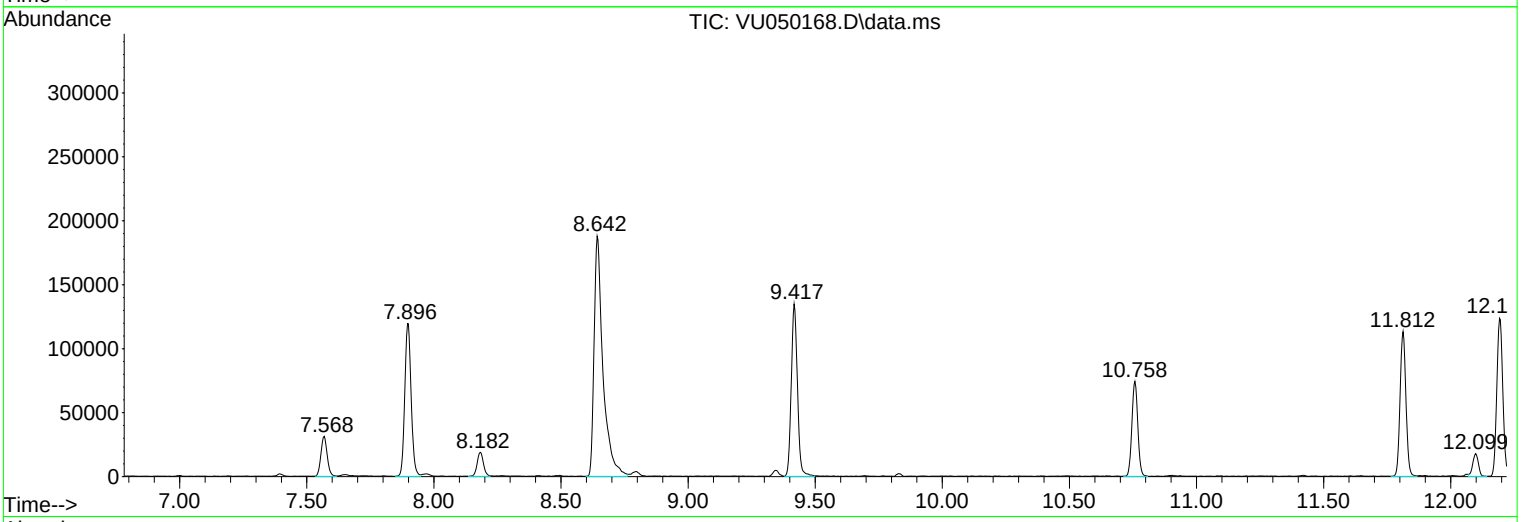
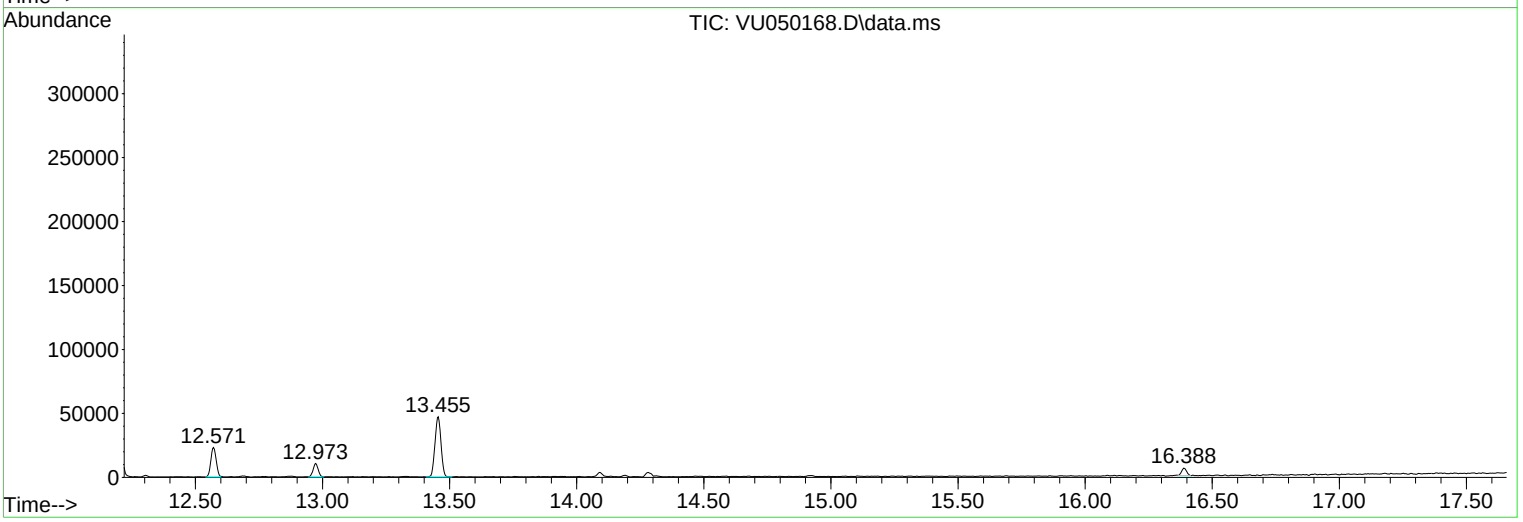
ClientSampleId :
DBUX9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.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

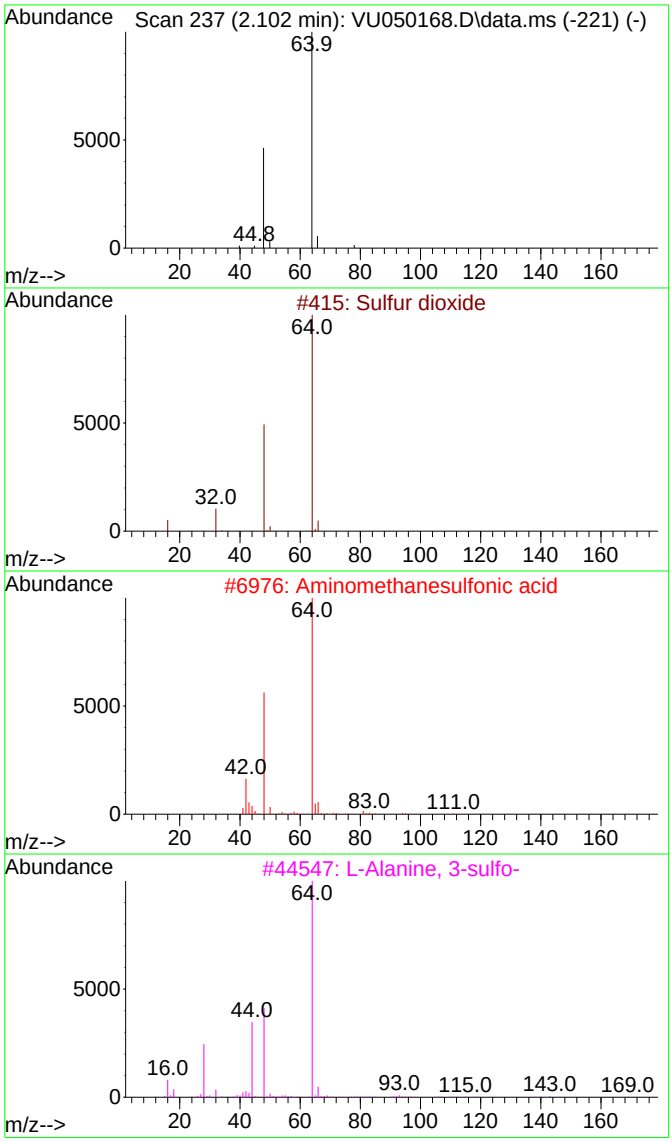
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

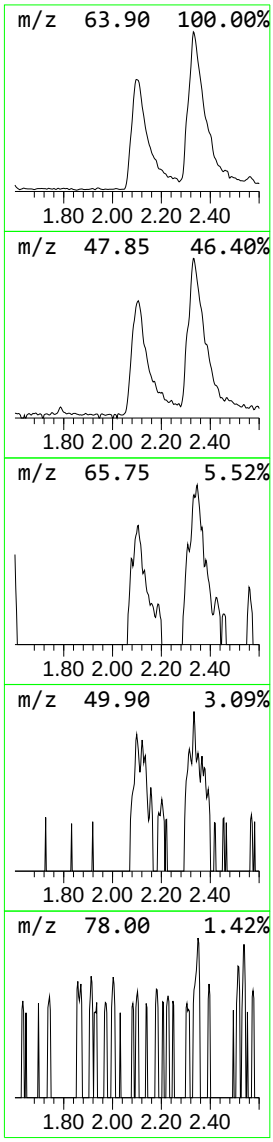
****

Peak Number 1 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.102	1.49 ug/L	52561	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	74
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5	Sulfur dioxide	64	O2S	007446-09-5	4





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Instrument :
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ClientSampleId :
DBUX9

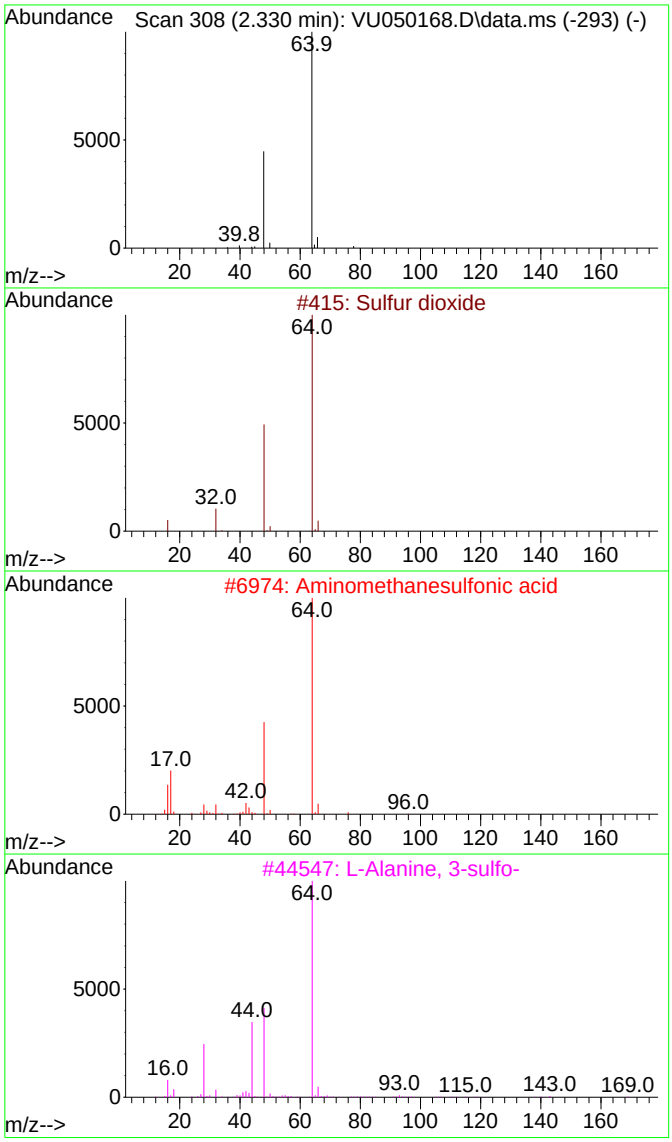
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

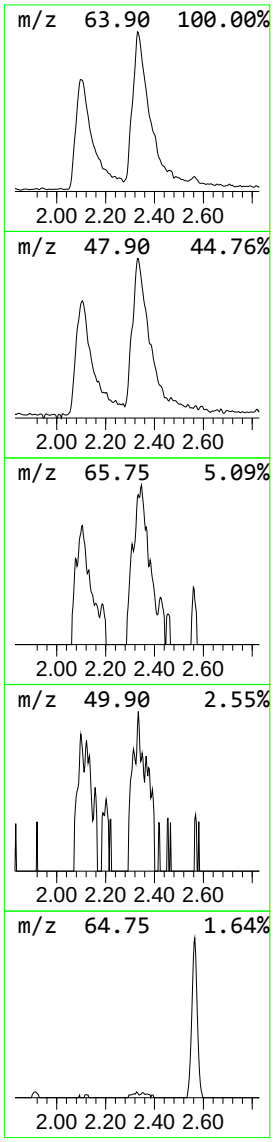
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Aminomethanesulfonic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.330	2.36 ug/L	83388	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfur dioxide	64	O2S	007446-09-5	90
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3	L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4	Sulfur dioxide	64	O2S	007446-09-5	5
5	Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5





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Instrument :
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ClientSampleId :
DBUX9

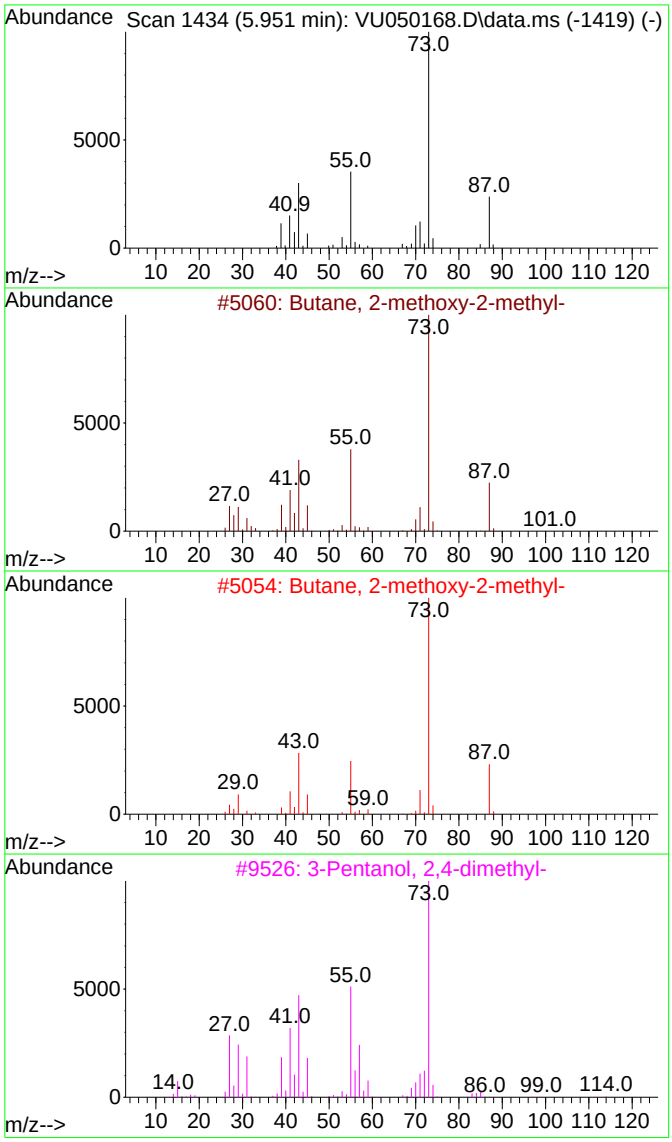
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

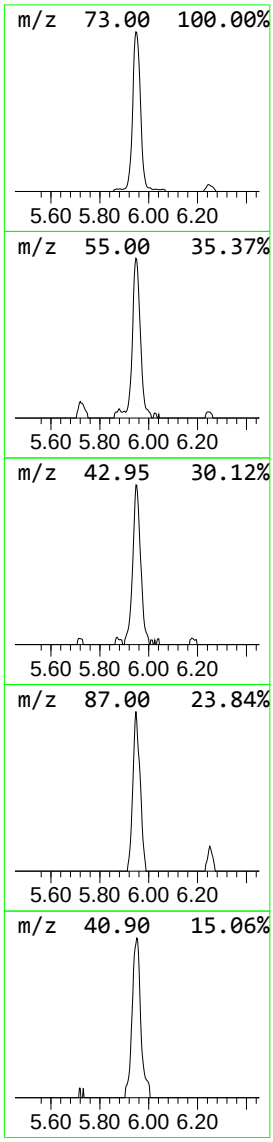
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.951	2.09 ug/L	74134	1,4-Difluorobenzene	6.250

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64
2	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	39
3	3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	28
4	Methane, isothiocyanato-	73	C2H3NS	000556-61-6	9
5	Morpholine	87	C4H9NO	000110-91-8	9





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ALS Vial : 41 Sample Multiplier: 1

Instrument :
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ClientSampleId :
DBUX9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

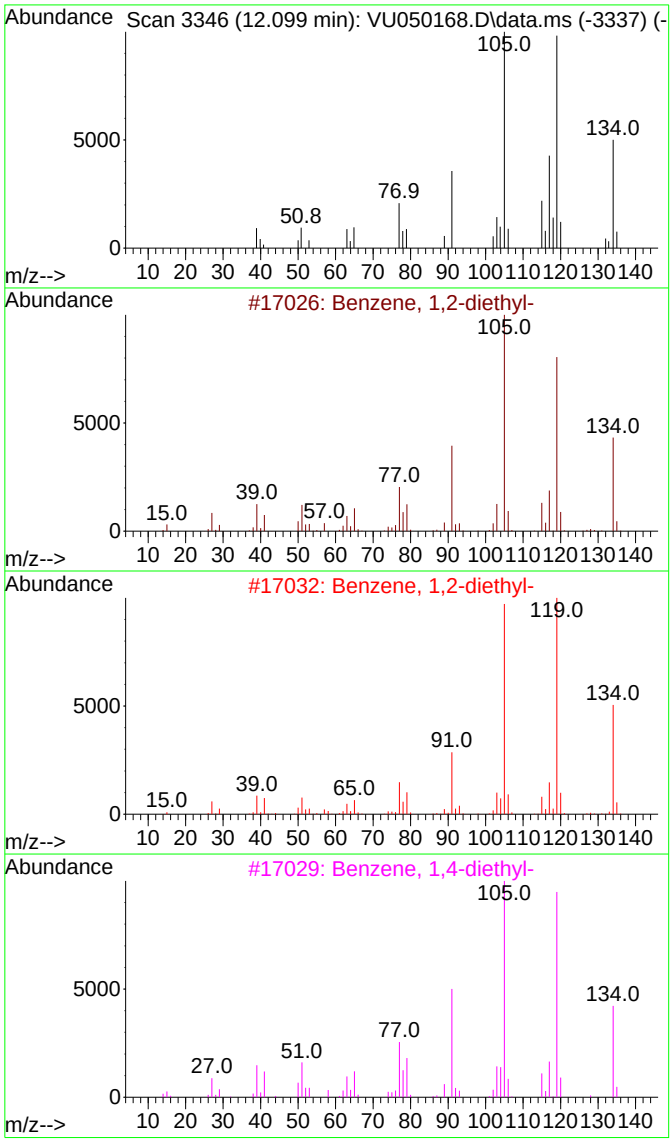
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

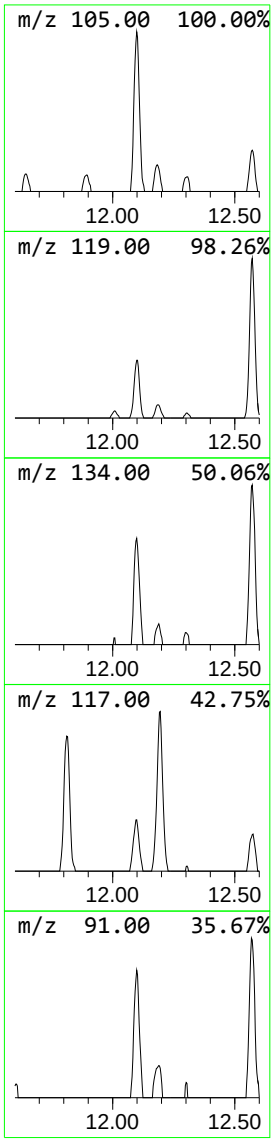
****

Peak Number 5 Benzene, 1,2-diethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.099	0.76 ug/L	27260	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	89
2	Benzene, 1,2-diethyl-	134	C10H14	000135-01-3	76
3	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	76
4	Benzene, 1,3-diethyl-	134	C10H14	000141-93-5	76
5	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	76





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Instrument :
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ClientSampleId :
DBUX9

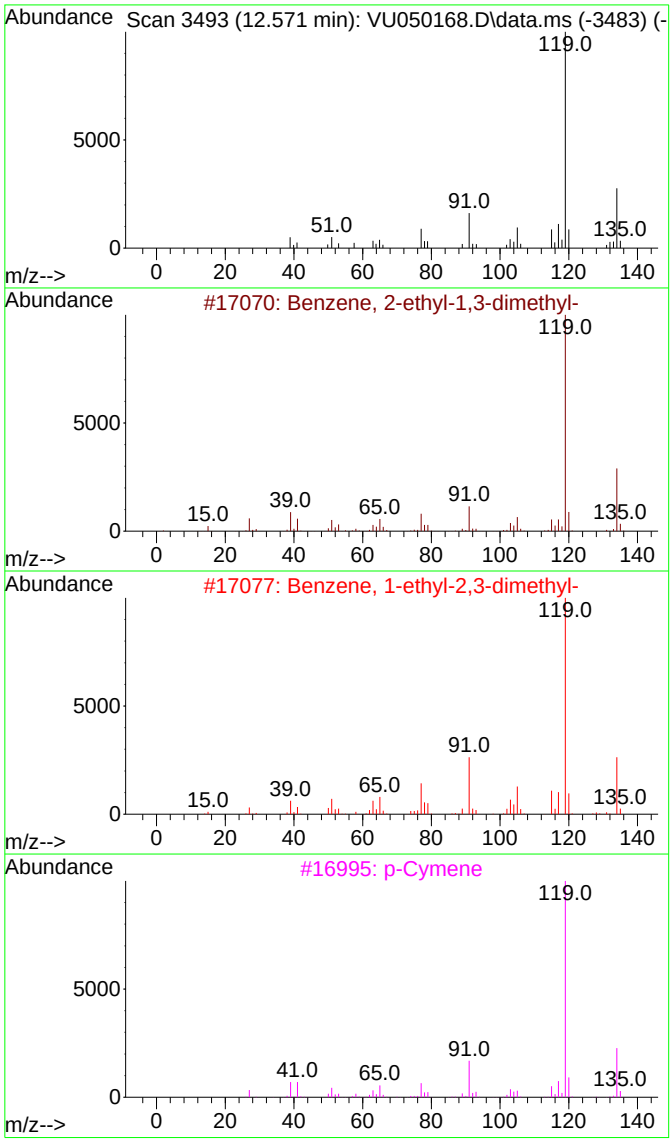
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080422WMA.M
Quant Title : TRACE VOA SFAM1.0

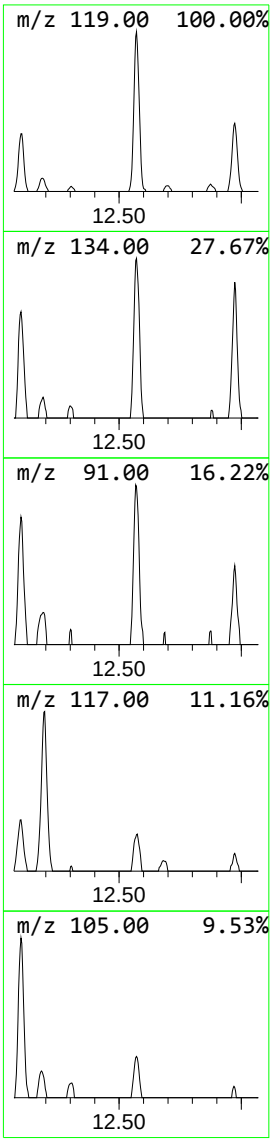
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 2-ethyl-1,3-dimethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.571	0.93 ug/L	33212	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
2	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	95
3	p-Cymene	134	C10H14	000099-87-6	95
4	Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	95
5	Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	94





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ALS Vial : 41 Sample Multiplier: 1

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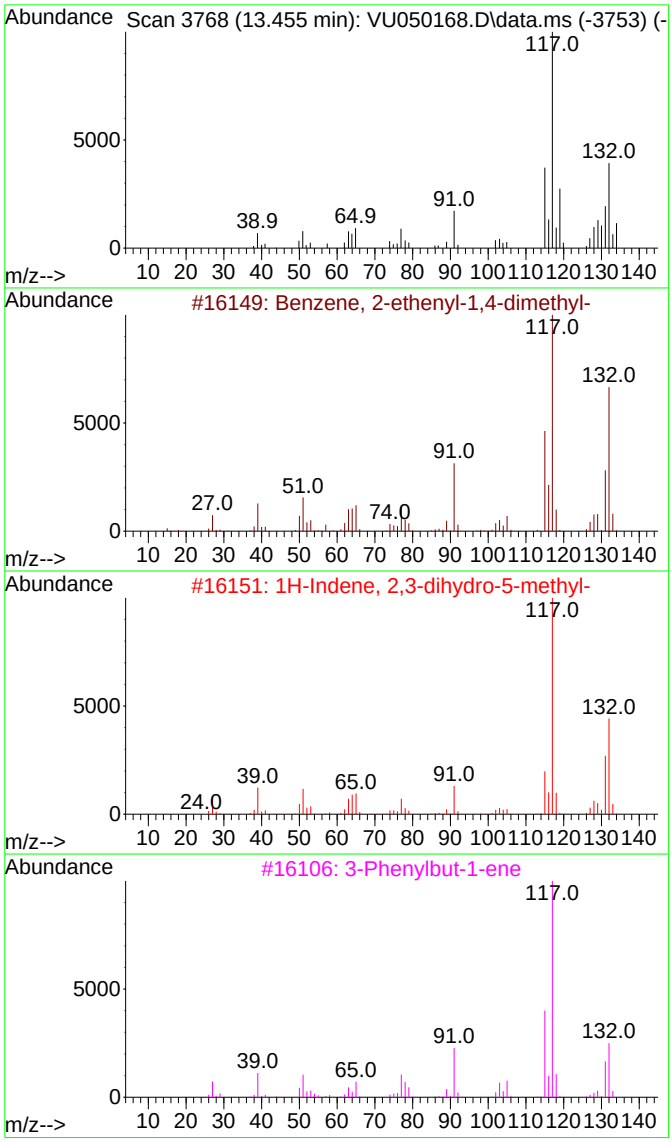
Quant Title : TRACE VOA SFAM1.0

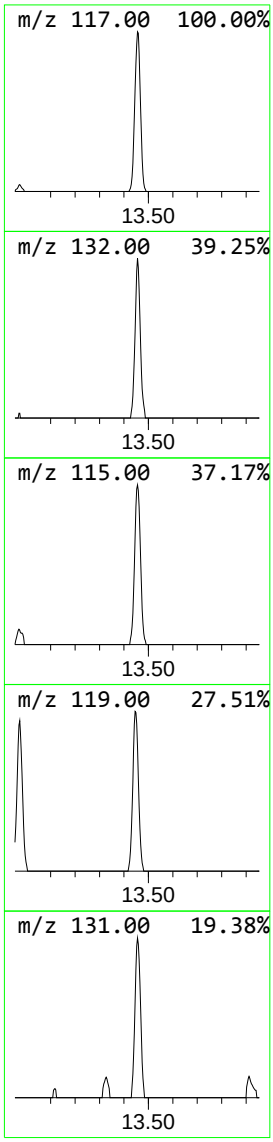
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.455	2.14 ug/L	76699	1,4-Dichlorobenzene-d4	11.812

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	91
2	1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	76
3	3-Phenylbut-1-ene	132	C10H12	000934-10-1	70
4	1H-Indene, 2,3-dihydro-2-methyl-	132	C10H12	000824-63-5	70
5	1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	68





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Sulfur dioxide	2.102	1.5	ug/L	52561	1	6.250	176957	5.0
Aminomethanesul...	2.330	2.4	ug/L	83388	1	6.250	176957	5.0
Butane, 2-metho...	5.951	2.1	ug/L	74134	1	6.250	176957	5.0
Benzene, 1,2-di...	12.099	0.8	ug/L	27260	3	11.812	178873	5.0
Benzene, 2-ethy...	12.571	0.9	ug/L	33212	3	11.812	178873	5.0
Benzene, 2-ethe...	13.455	2.1	ug/L	76699	3	11.812	178873	5.0