

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
 Data File : VU051531.D
 Acq On : 27 Oct 2022 03:48
 Operator : JC/MD
 Sample : N5300-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 39 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHA72

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\SFAMUTR100722WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU051531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.372	309	321	341	rBV	13702089	20004598	3.50%	1.083%
2	3.993	801	825	849	rBV2	34925884	92039833	16.09%	4.981%
3	5.044	1137	1152	1173	rBV	2710458	6256078	1.09%	0.339%
4	5.832	1347	1397	1410	rBV6	118760251	571965764	100.00%	30.953%
5	9.455	2500	2524	2550	rBV3	68528334	132859777	23.23%	7.190%
6	9.574	2550	2561	2570	rVV2	22185062	39281479	6.87%	2.126%
7	9.623	2570	2576	2586	rVV	13608783	19323650	3.38%	1.046%
8	9.732	2586	2610	2633	rVB5	127989374	433382894	75.77%	23.453%
9	10.115	2713	2729	2752	rVB3	76165069	142944609	24.99%	7.736%
10	10.484	2830	2844	2856	rBV	8751465	13603465	2.38%	0.736%
11	10.896	2958	2972	2989	rBV2	21168880	38900219	6.80%	2.105%
12	10.999	2990	3004	3021	rBV2	28681968	46206885	8.08%	2.501%
13	11.092	3021	3033	3043	rBV	17425549	26553387	4.64%	1.437%
14	11.291	3084	3095	3117	rVB	15345798	24218405	4.23%	1.311%
15	11.475	3138	3152	3168	rBV3	56580072	93094282	16.28%	5.038%
16	11.835	3257	3264	3272	rVV	4954670	8096818	1.42%	0.438%
17	11.893	3272	3282	3311	rVV2	29563410	52716811	9.22%	2.853%
18	12.095	3332	3345	3363	rVV2	15950882	26919338	4.71%	1.457%
19	12.189	3363	3374	3396	rVB4	4184722	8758427	1.53%	0.474%
20	12.481	3448	3465	3484	rBV	24976000	50721351	8.87%	2.745%

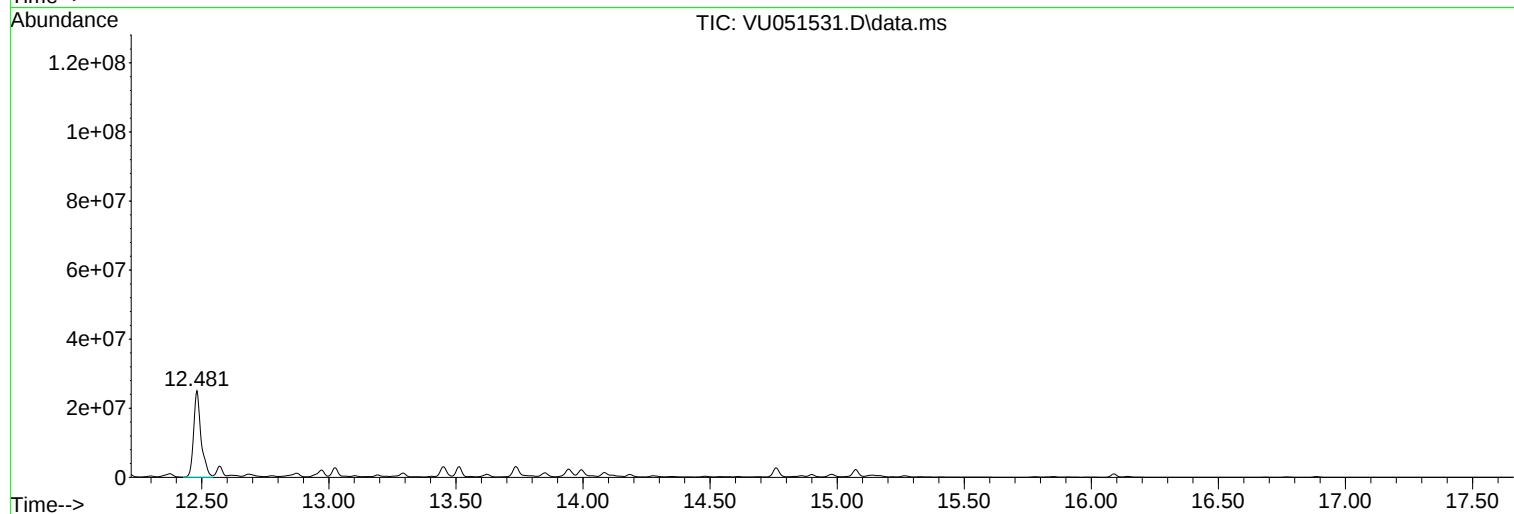
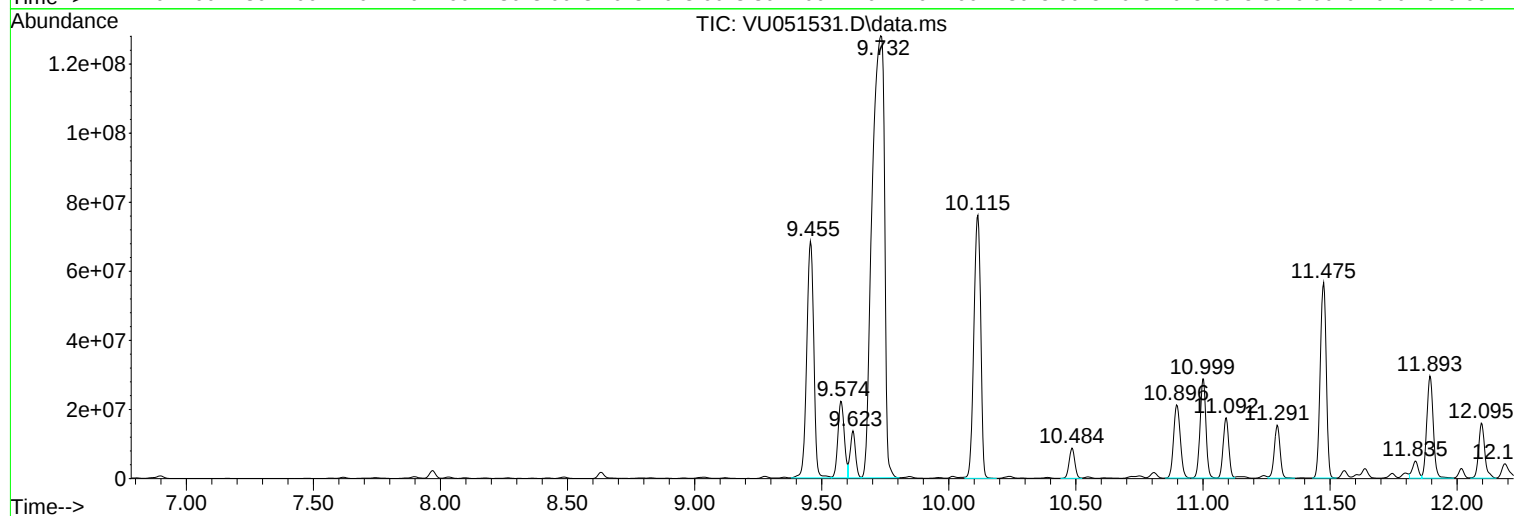
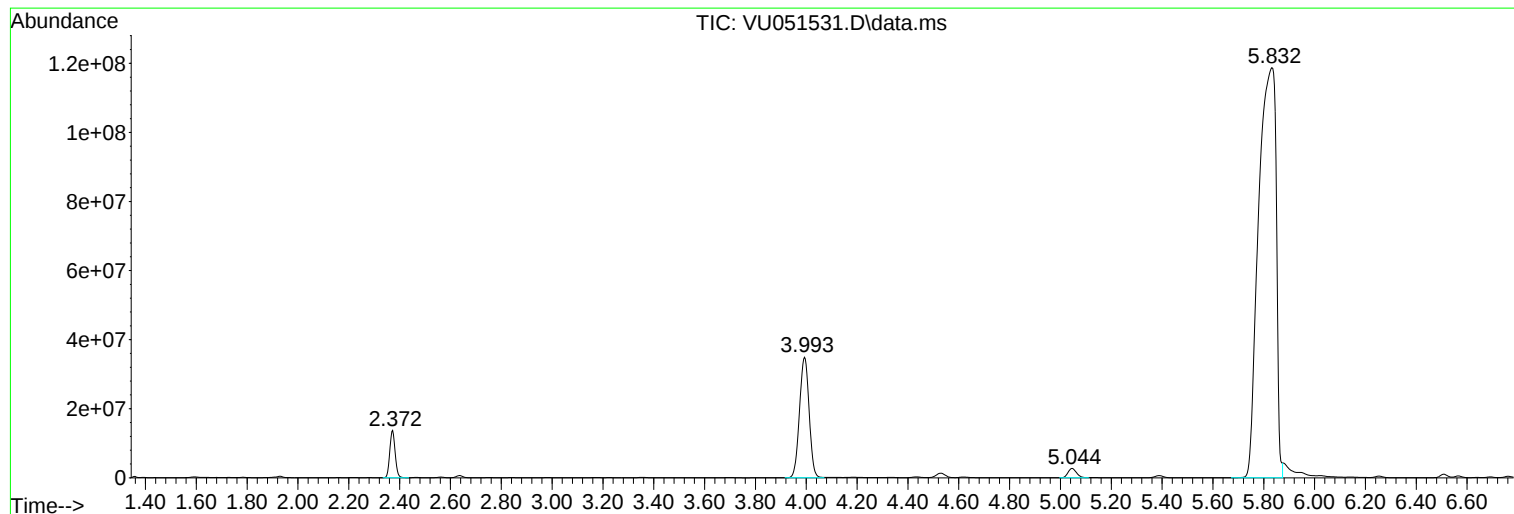
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ClientSampleId :
BHA72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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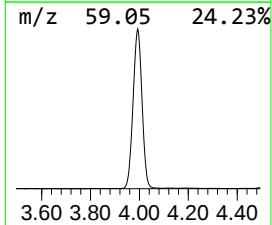
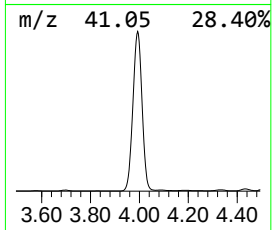
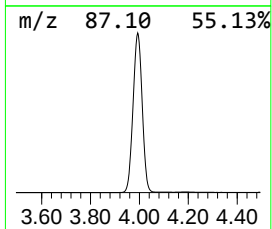
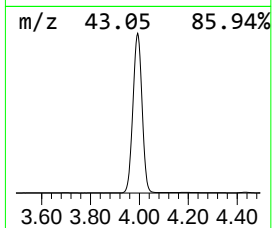
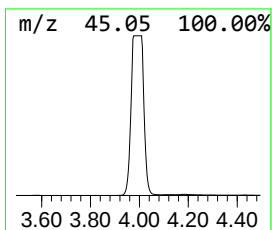
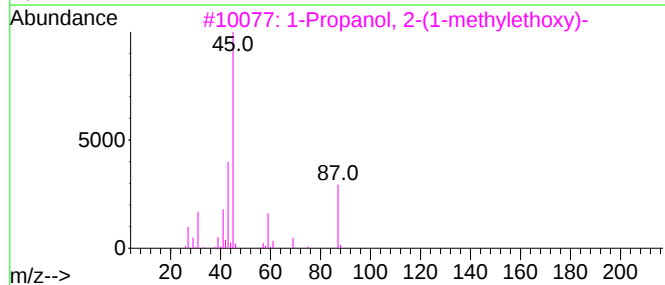
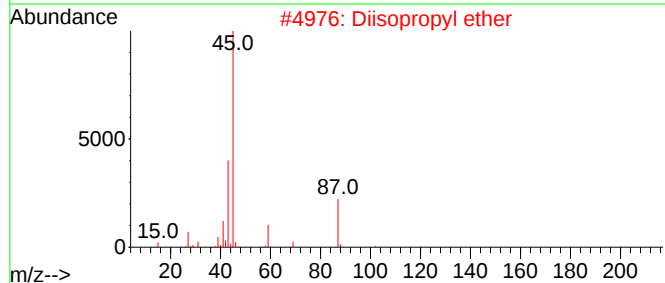
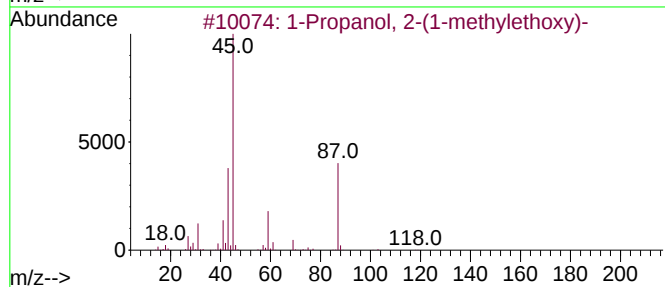
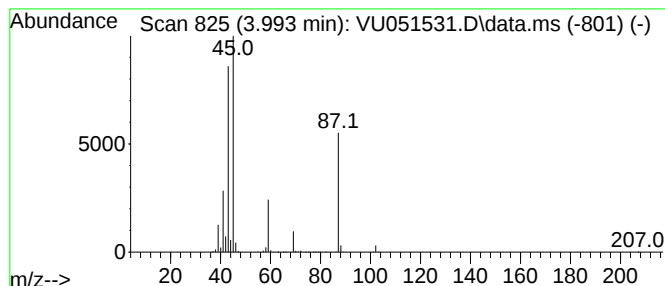
Instrument :
MSVOA_U
ClientSampleId :
BHA72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 1-Propanol, 2-(1-methyletho... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.993	0.80 ug/L	92039800	1,4-Difluorobenzene	6.250	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	72
2	Diisopropyl ether	102	C6H14O	000108-20-3	72
3	1-Propanol, 2-(1-methylethoxy)-	118	C6H14O2	003944-37-4	56
4	Diisopropyl ether	102	C6H14O	000108-20-3	46
5	Diisopropyl ether	102	C6H14O	000108-20-3	37



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Instrument :
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ClientSampleId :
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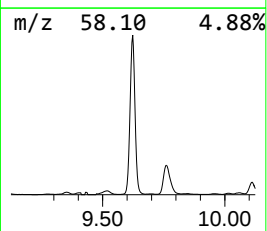
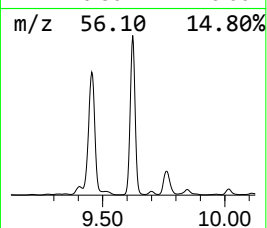
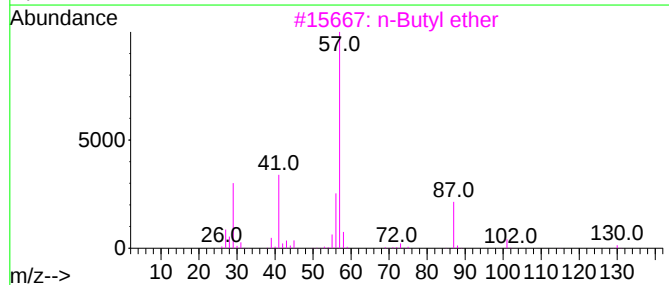
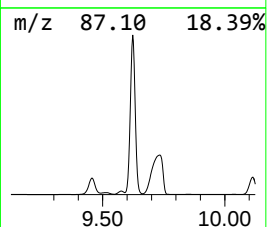
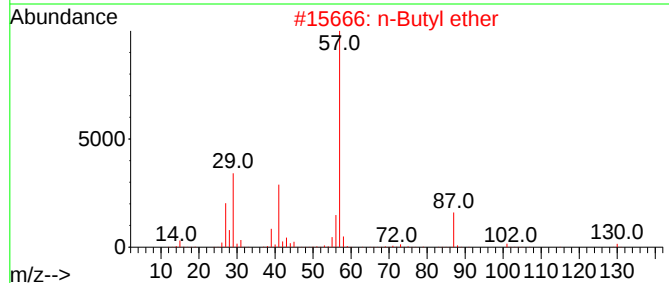
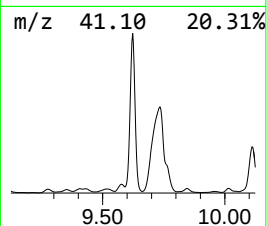
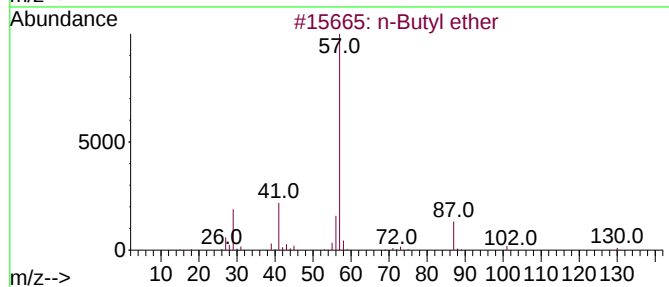
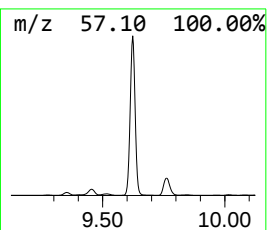
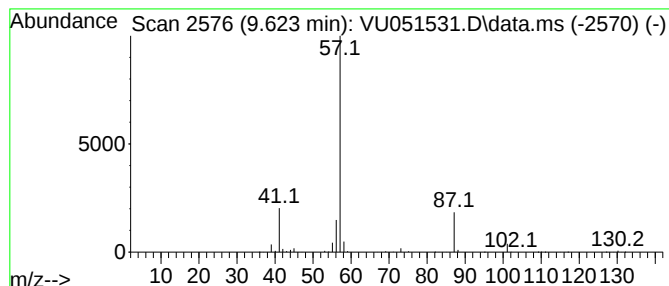
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 n-Butyl ether Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.623	0.73 ug/L	19323700	Chlorobenzene-d5	9.423

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Butyl ether			130	C8H18O	000142-96-1	78
2	n-Butyl ether			130	C8H18O	000142-96-1	72
3	n-Butyl ether			130	C8H18O	000142-96-1	64
4	n-Butyl ether			130	C8H18O	000142-96-1	59
5	Ethanol, 2-butoxy-			118	C6H14O2	000111-76-2	56



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ALS Vial : 39 Sample Multiplier: 1

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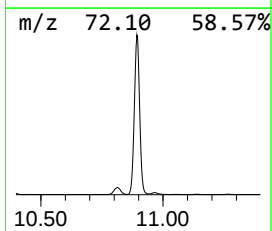
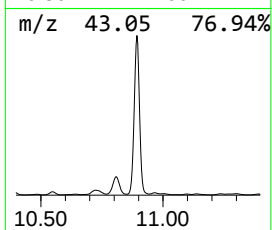
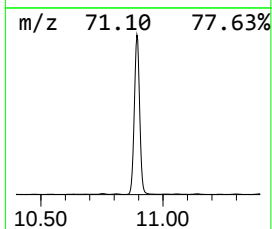
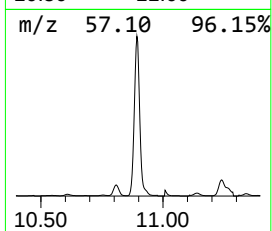
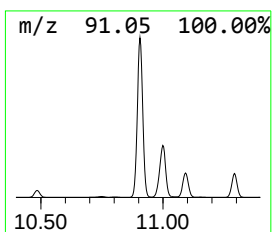
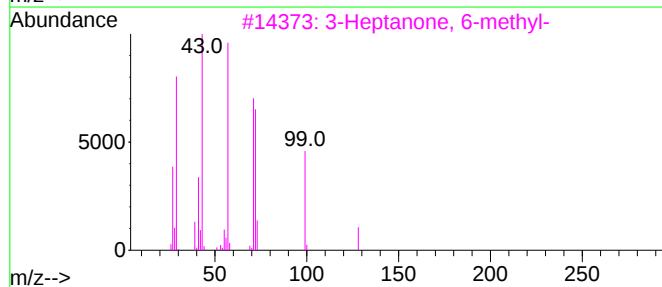
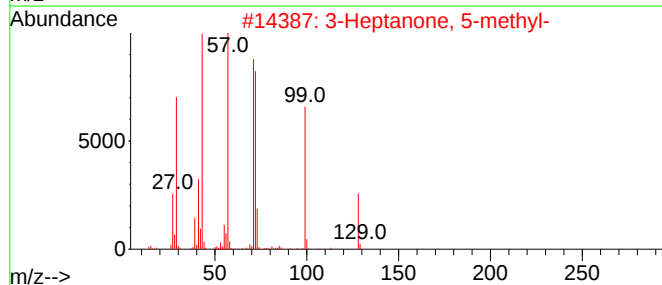
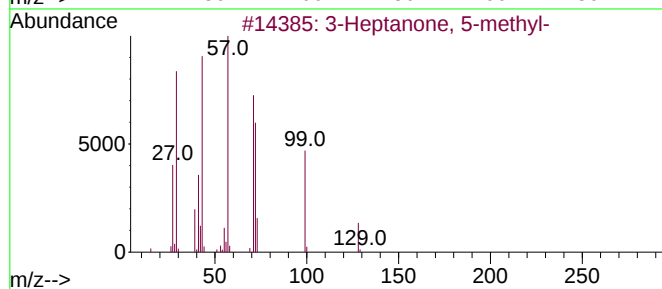
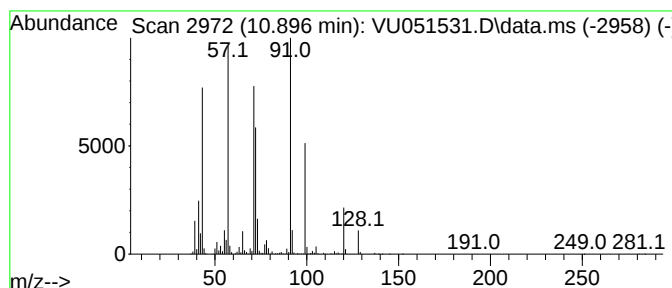
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 3-Heptanone, 5-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.896	24.02 ug/L	38900200	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	94
2			3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	89
3			3-Heptanone, 6-methyl-	128	C8H16O	000624-42-0	76
4			3-Octanone	128	C8H16O	000106-68-3	76
5			3-Heptanone, 5-methyl-	128	C8H16O	000541-85-5	76



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Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

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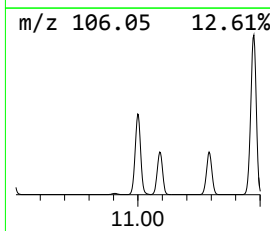
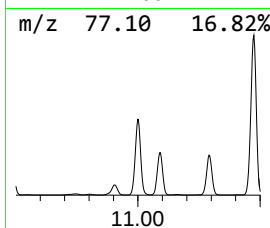
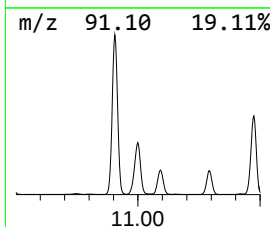
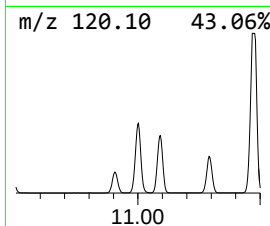
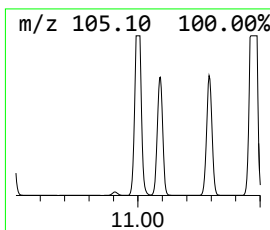
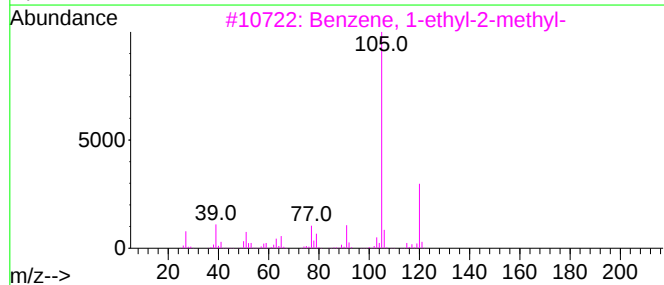
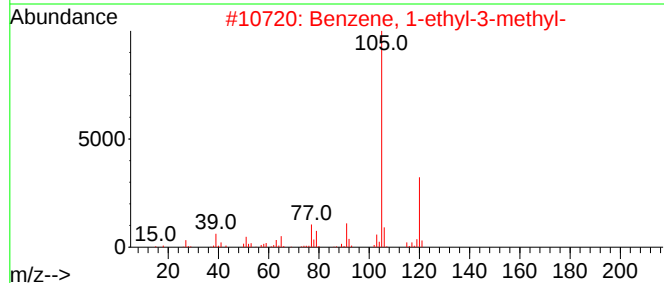
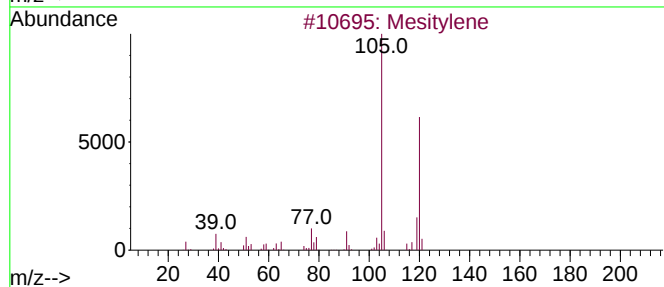
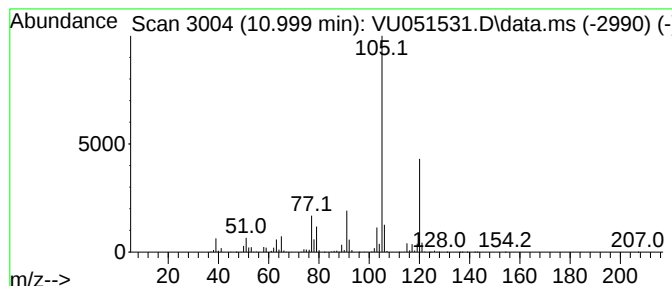
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Benzene, 1-ethyl-3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.999	28.53 ug/L	46206900	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	91
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
3			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
4			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	90
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90



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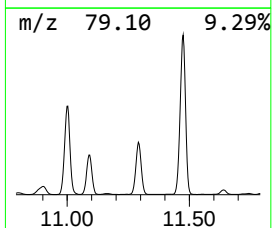
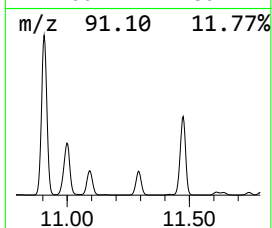
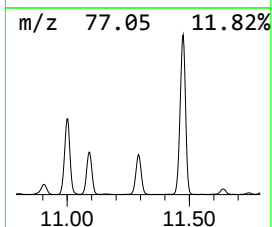
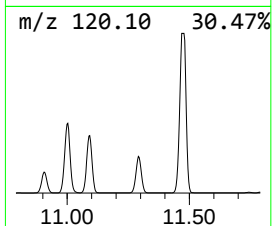
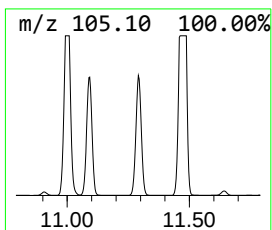
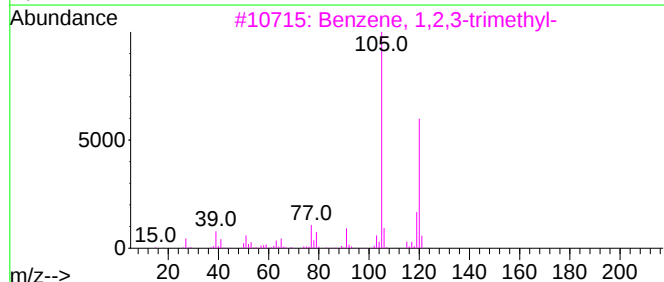
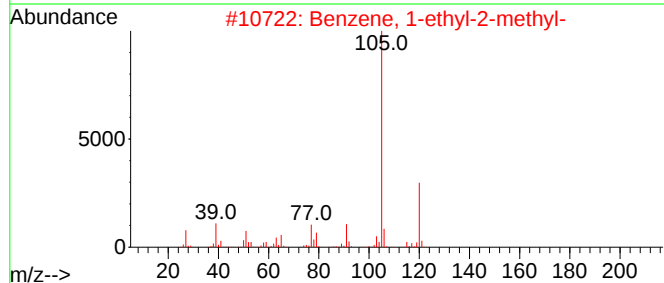
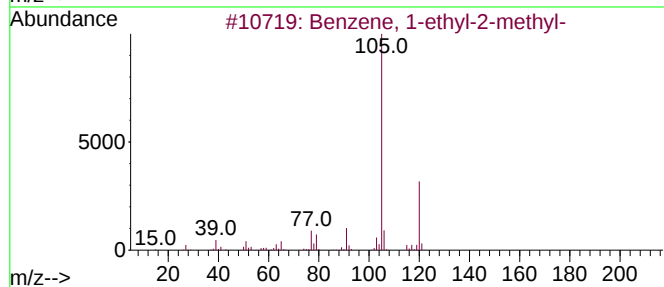
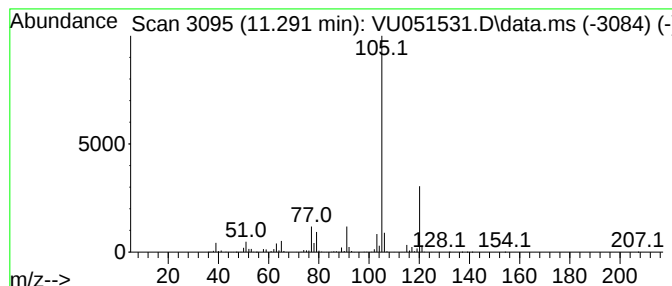
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 6 Benzene, 1-ethyl-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.291	14.96 ug/L	24218400	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
3			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91



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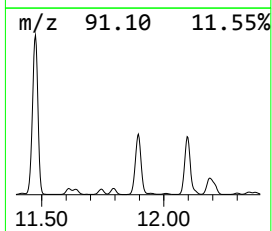
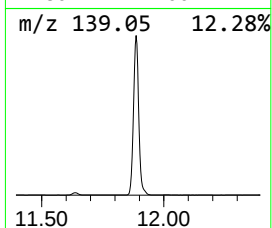
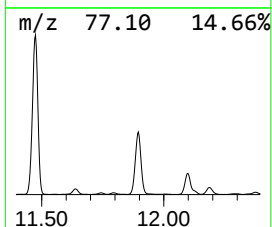
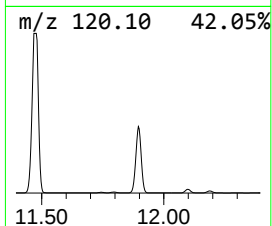
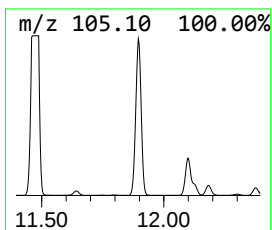
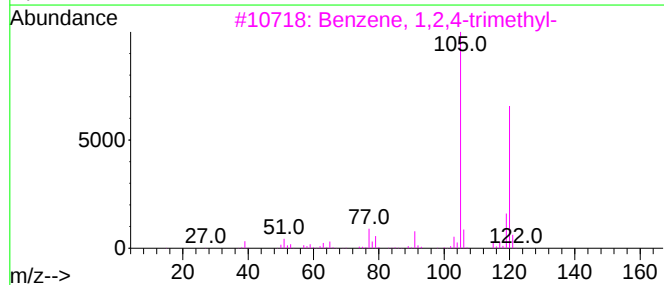
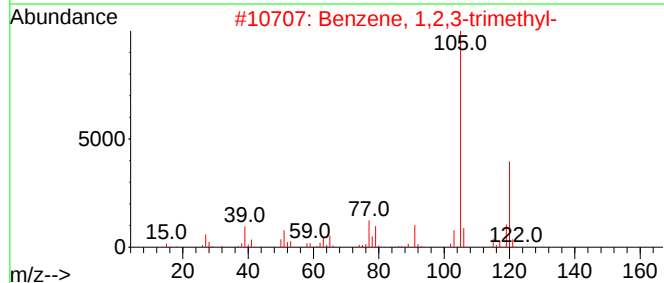
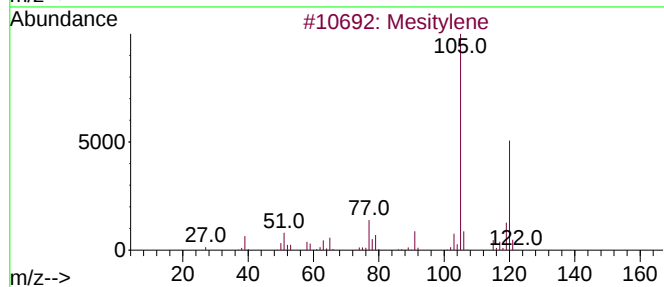
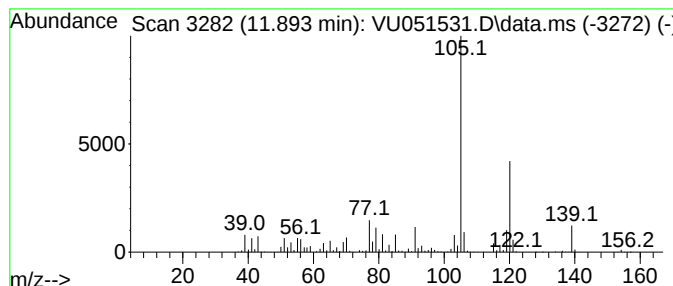
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.893	32.55 ug/L	52716800	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	95
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	94
4			Mesitylene	120	C9H12	000108-67-8	93
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051531.D
Acq On : 27 Oct 2022 03:48
Operator : JC/MD
Sample : N5300-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA72

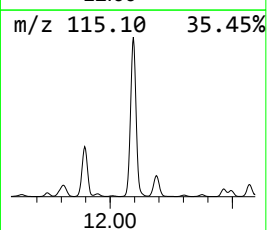
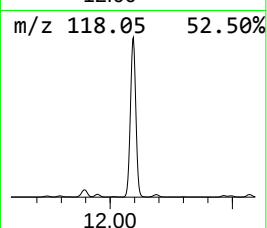
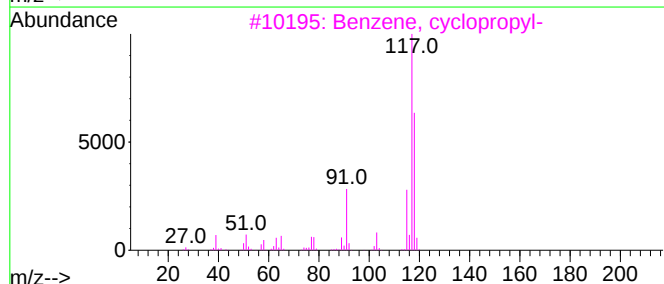
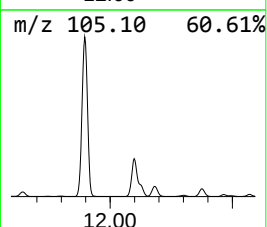
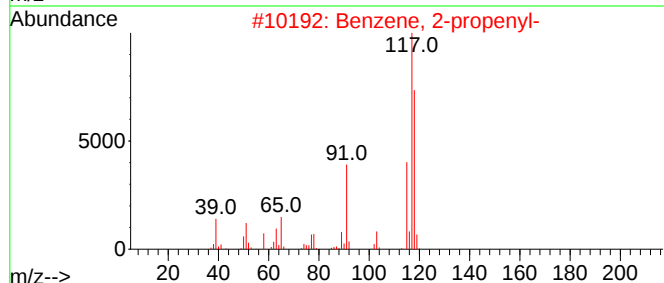
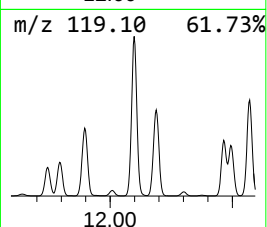
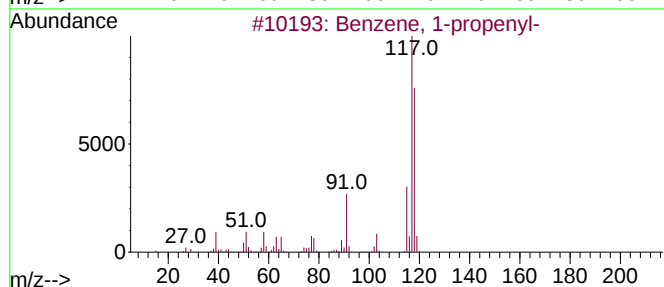
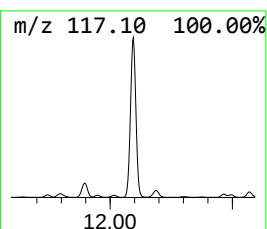
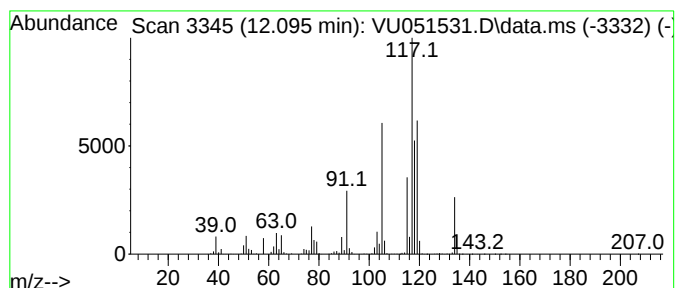
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Benzene, 1-propenyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.095	16.62 ug/L	26919300	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-propenyl-	118	C9H10	000637-50-3	60
2			Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
3			Benzene, cyclopropyl-	118	C9H10	000873-49-4	60
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	60
5			(Z)-1-Phenylpropene	118	C9H10	000766-90-5	55



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051531.D
Acq On : 27 Oct 2022 03:48
Operator : JC/MD
Sample : N5300-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

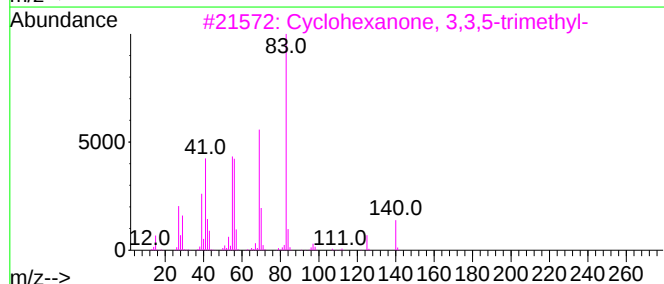
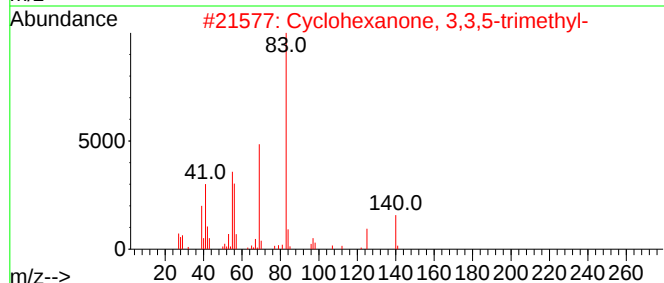
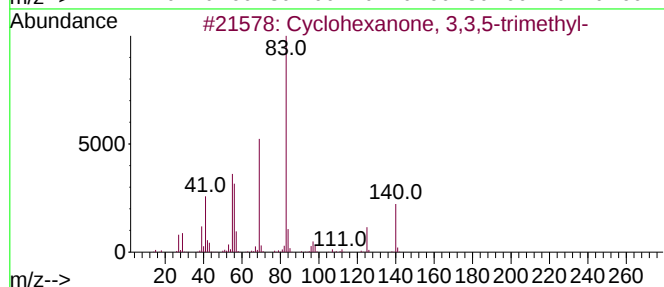
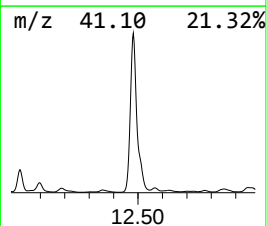
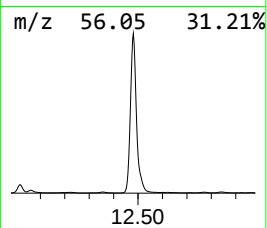
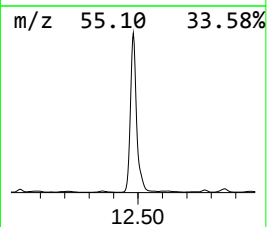
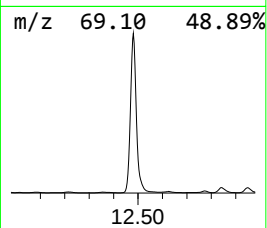
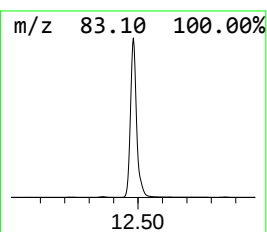
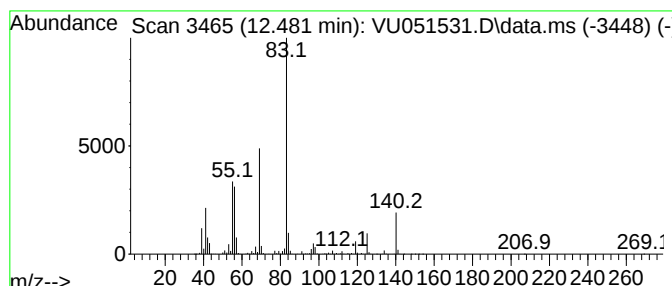
Instrument :
MSVOA_U
ClientSampleId :
BHA72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 9 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD			R.T.
12.481	31.32 ug/L	50721400	1,4-Dichlorobenzene-d4			11.812
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Cyclohexanone, 3,3,5-trimethyl-		140	C9H16O	000873-94-9	96
2	Cyclohexanone, 3,3,5-trimethyl-		140	C9H16O	000873-94-9	95
3	Cyclohexanone, 3,3,5-trimethyl-		140	C9H16O	000873-94-9	91
4	Cyclohexanone, 3,3,5-trimethyl-		140	C9H16O	000873-94-9	91
5	2,4,6-Trimethyl-3-heptene		140	C10H20	1000113-56-9	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102622\
Data File : VU051531.D
Acq On : 27 Oct 2022 03:48
Operator : JC/MD
Sample : N5300-01
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 39 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BHA72

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100722WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol, 2-(...	3.993	0.8	ug/L	92039800	1	6.250	571966000	5.0
n-Butyl ether	9.623	0.7	ug/L	19323700	2	9.423	132860000	5.0
3-Heptanone, 5-...	10.896	24.0	ug/L	38900200	3	11.812	8096820	5.0
Benzene, 1-ethy...	10.999	28.5	ug/L	46206900	3	11.812	8096820	5.0
Benzene, 1-ethy...	11.291	15.0	ug/L	24218400	3	11.812	8096820	5.0
Benzene, 1,2,3-...	11.893	32.5	ug/L	52716800	3	11.812	8096820	5.0
Benzene, 1-prop...	12.095	16.6	ug/L	26919300	3	11.812	8096820	5.0
Cyclohexanone, ...	12.481	31.3	ug/L	50721400	3	11.812	8096820	5.0