

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU070124\
Data File : VU059709.D
Acq On : 02 Jul 2024 01:16
Operator : MD/SY
Sample : P3121-11
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 42 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BJ6

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: VU059709.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.785	144	154	178	rBV	518962	804581	2.92%	2.316%
2	4.653	1028	1046	1124	rBV	12243609	27527160	100.00%	79.248%
3	5.717	1354	1377	1406	rBV4	212814	563938	2.05%	1.624%
4	6.242	1527	1540	1563	rBV	242595	471193	1.71%	1.357%
5	6.534	1618	1631	1663	rBV	198744	382451	1.39%	1.101%
6	7.891	2039	2053	2069	rBV	267134	463328	1.68%	1.334%
7	8.627	2273	2282	2317	rVB	320794	643294	2.34%	1.852%
8	9.412	2513	2526	2543	rBV	355078	597442	2.17%	1.720%
9	11.566	3184	3196	3212	rBV	218705	362395	1.32%	1.043%
10	11.804	3259	3270	3288	rVB	394678	646891	2.35%	1.862%
11	12.187	3377	3389	3410	rVB	306261	504711	1.83%	1.453%
12	12.765	3557	3569	3576	rBV	893972	1291914	4.69%	3.719%
13	12.807	3576	3582	3599	rVB	274068	476199	1.73%	1.371%

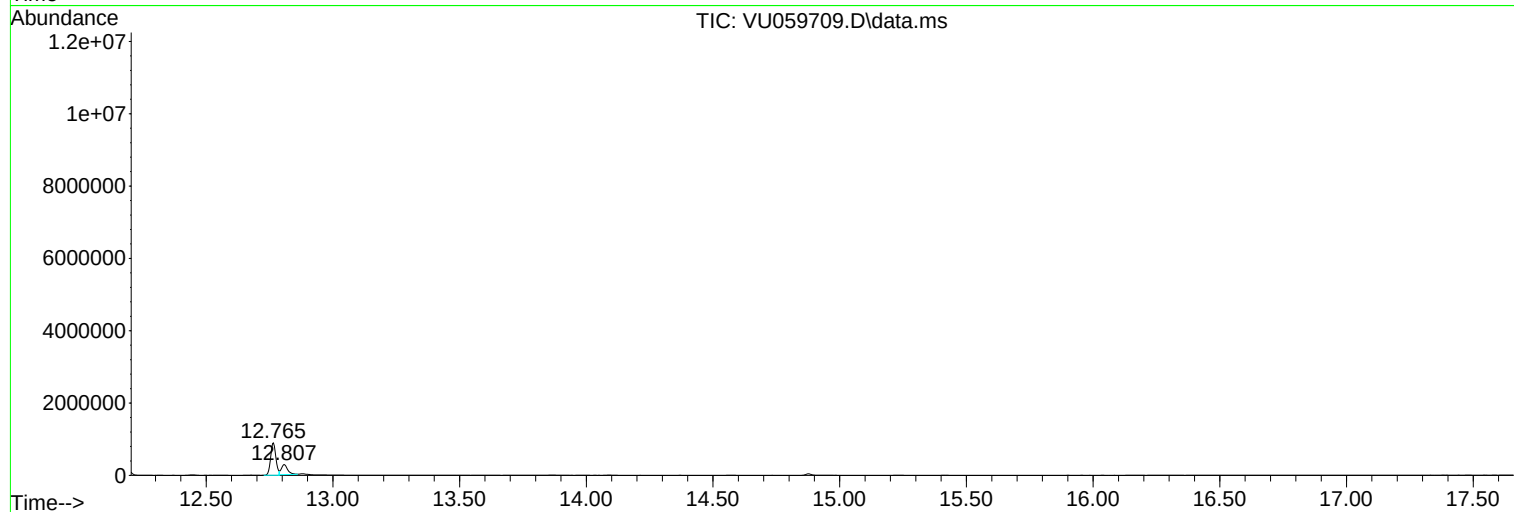
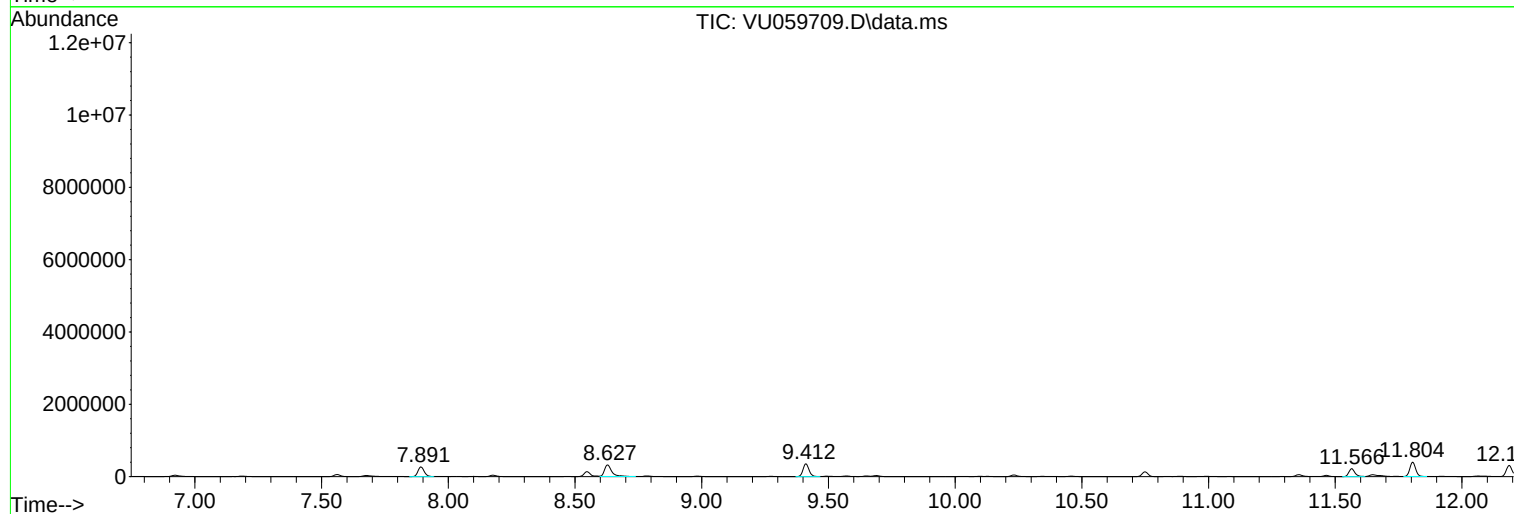
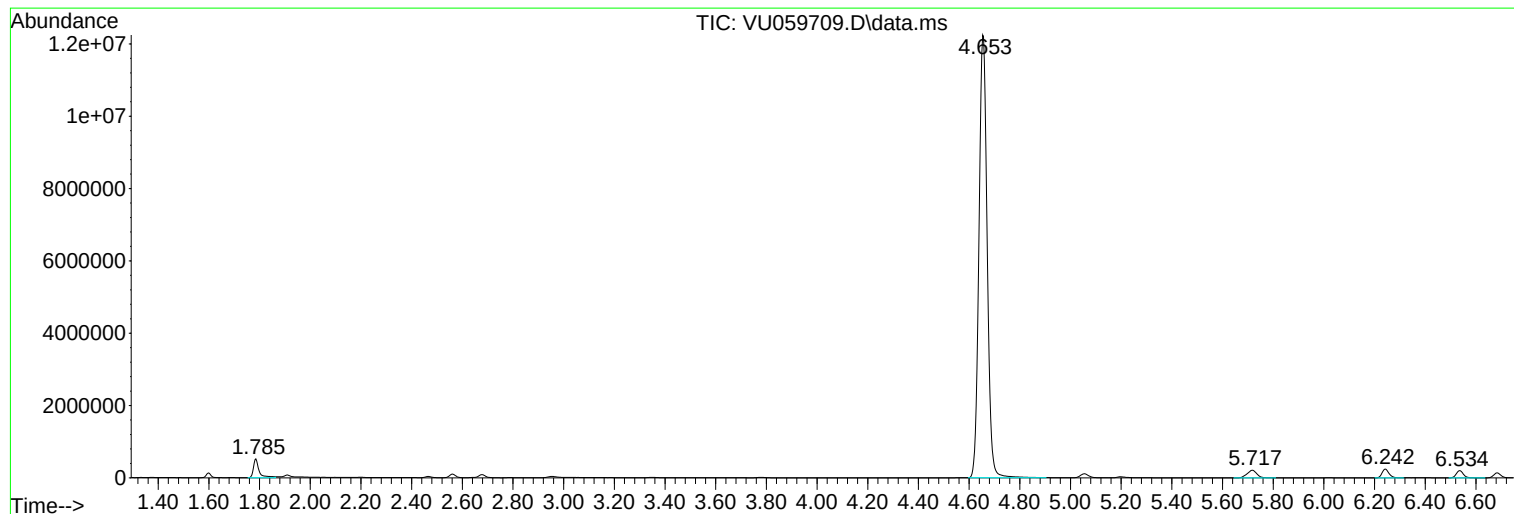
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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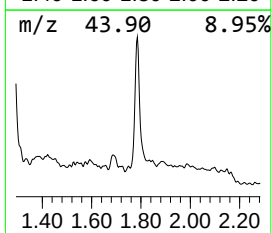
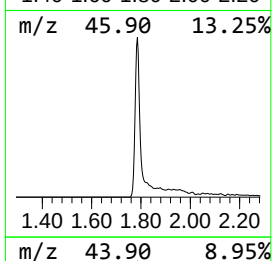
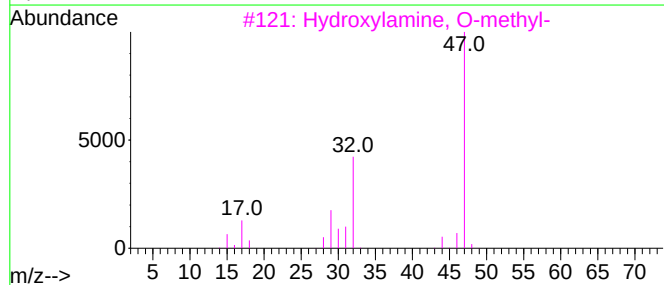
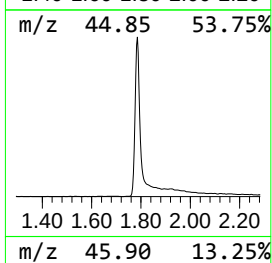
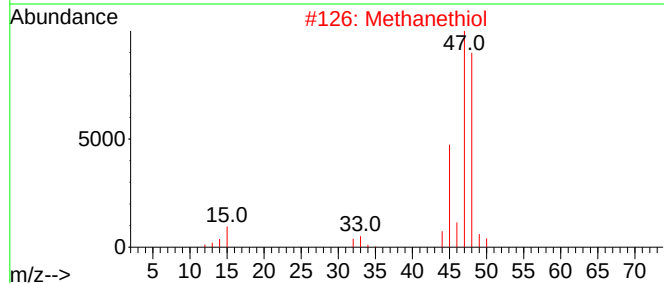
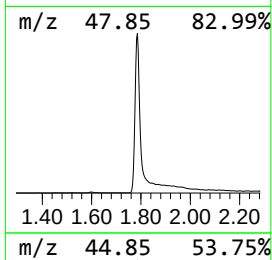
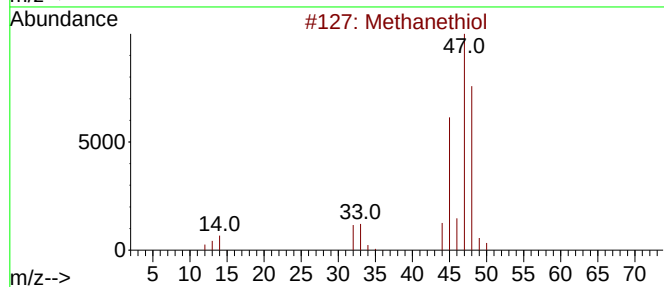
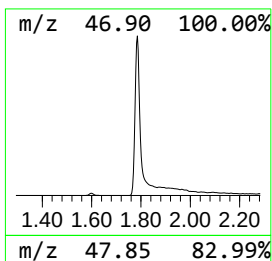
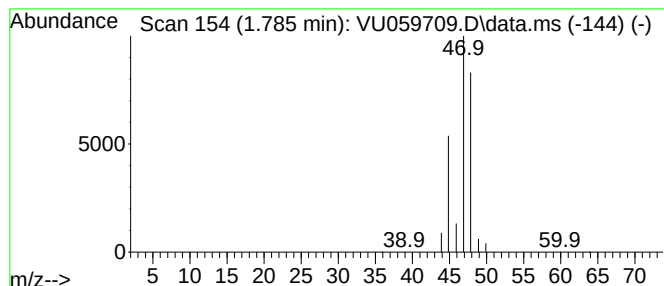
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Methanethiol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.785	8.54 ug/L	804581	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methanethiol	48	CH4S	000074-93-1	90
2			Methanethiol	48	CH4S	000074-93-1	90
3			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
4			Hydroxylamine, O-methyl-	47	CH5NO	000067-62-9	7
5			Methane, nitroso-	45	CH3NO	000865-40-7	5



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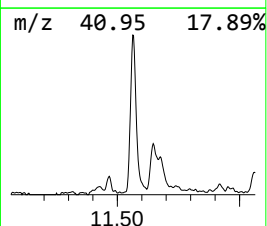
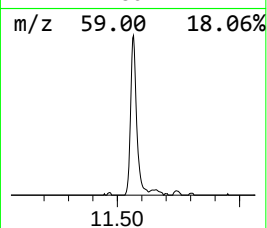
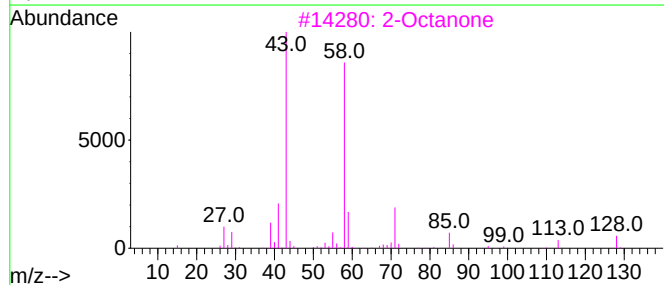
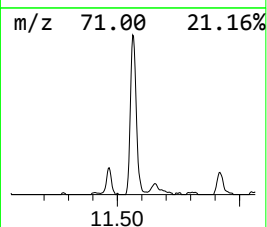
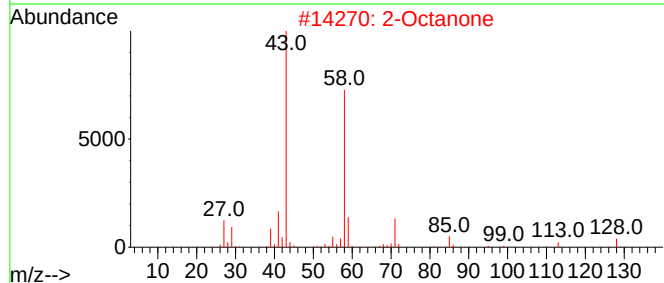
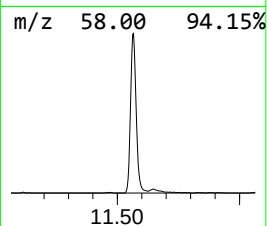
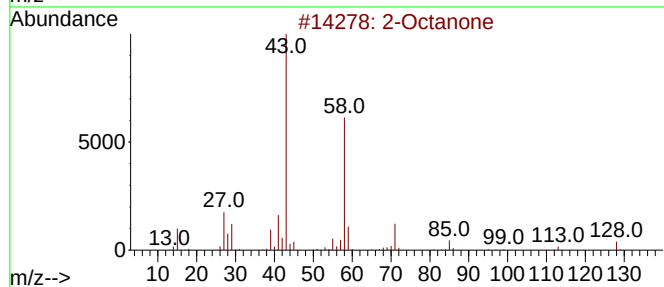
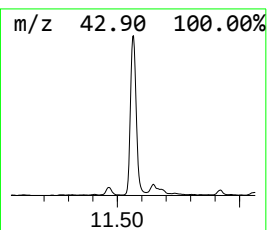
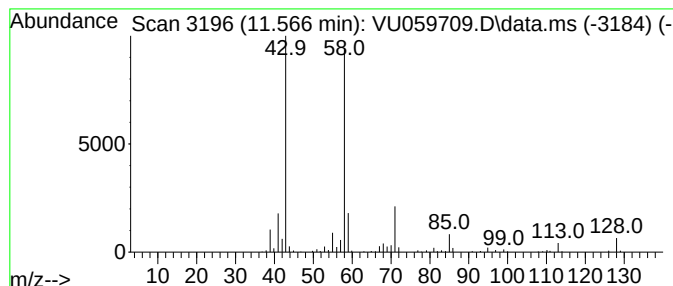
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2-Octanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.566	2.80 ug/L	362395	1,4-Dichlorobenzene-d4	11.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Octanone			128	C8H16O	000111-13-7	91
2	2-Octanone			128	C8H16O	000111-13-7	91
3	2-Octanone			128	C8H16O	000111-13-7	91
4	2-Octanone			128	C8H16O	000111-13-7	91
5	2-Octanone			128	C8H16O	000111-13-7	74



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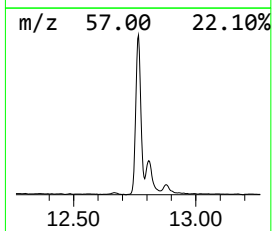
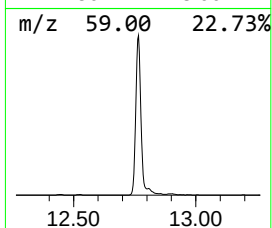
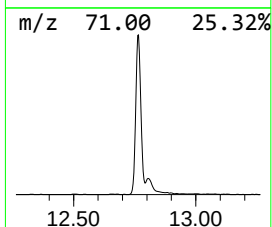
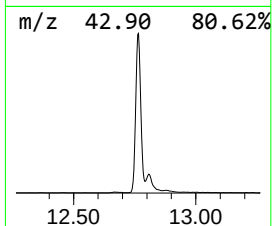
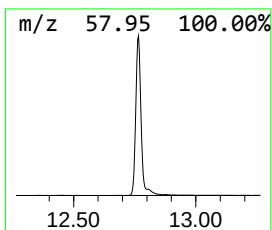
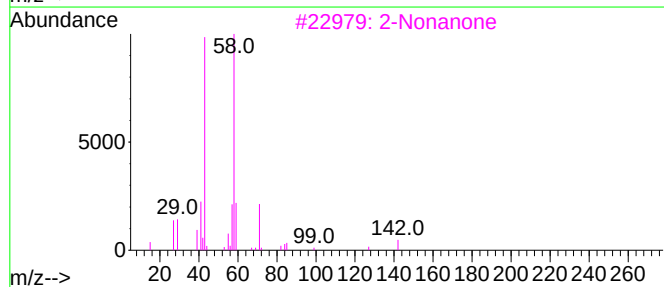
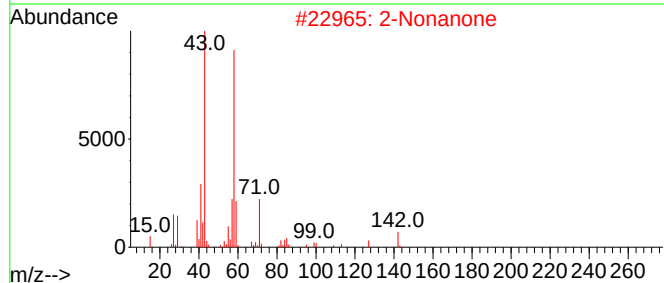
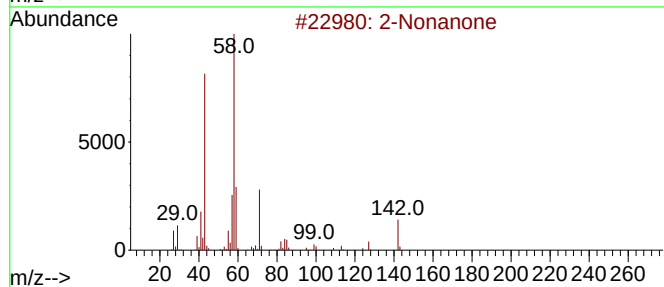
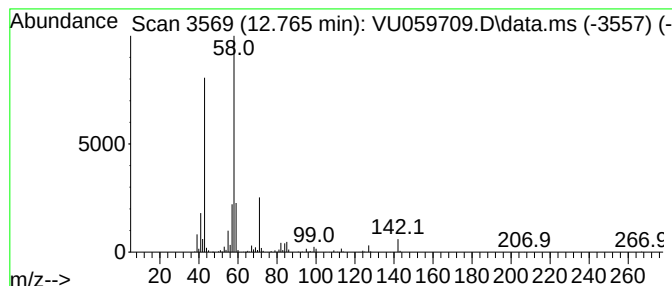
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2-Nonanone Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.765	9.99 ug/L	1291910	1,4-Dichlorobenzene-d4	11.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Nonanone			142	C9H18O	000821-55-6	91
2	2-Nonanone			142	C9H18O	000821-55-6	91
3	2-Nonanone			142	C9H18O	000821-55-6	87
4	2-Octanone			128	C8H16O	000111-13-7	72
5	2,4(3H,5H)-Furandione, 5-hexyl-5...			198	C11H18O3	054852-79-8	64



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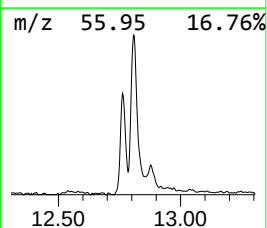
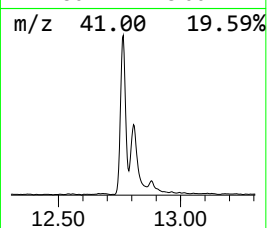
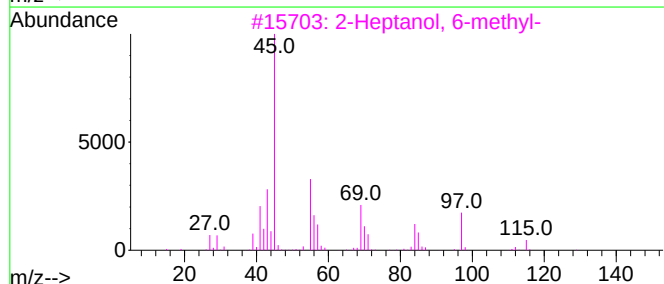
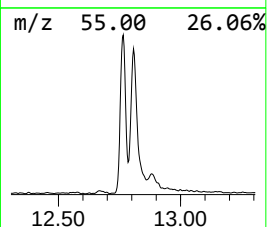
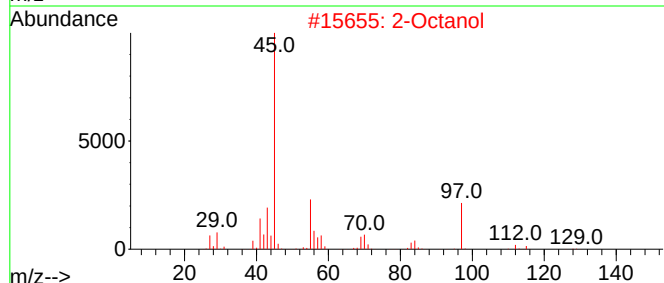
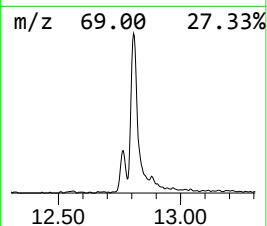
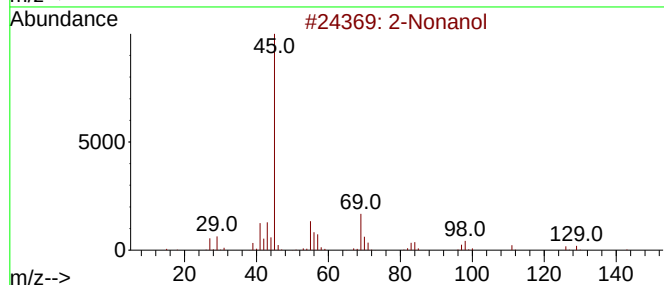
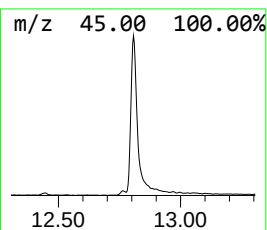
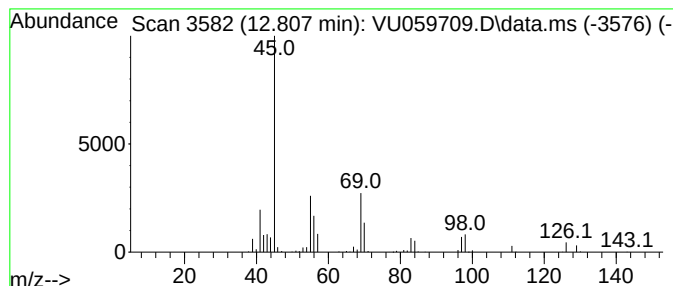
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 2-Nonanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.807	3.68 ug/L	476199	1,4-Dichlorobenzene-d4	11.804

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Nonanol	144	C9H20O	000628-99-9	78
2			2-Octanol	130	C8H18O	000123-96-6	72
3			2-Heptanol, 6-methyl-	130	C8H18O	004730-22-7	72
4			2-Octanol, (S)-	130	C8H18O	006169-06-8	64
5			2-Octanol	130	C8H18O	000123-96-6	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Methanethiol	1.785	8.5	ug/L	804581	1	6.242	471193	5.0
2-Octanone	11.566	2.8	ug/L	362395	3	11.804	646891	5.0
2-Nonanone	12.765	10.0	ug/L	1291910	3	11.804	646891	5.0
2-Nonanol	12.807	3.7	ug/L	476199	3	11.804	646891	5.0