

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062023\
 Data File : VU054616.D
 Acq On : 20 Jun 2023 17:34
 Operator : MD/SY
 Sample : 03258-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DCGX0

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\SFAMUTR060723WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU054616.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	43	58	100	rVB	11036330	35629441	100.00%	81.445%
2	2.589	395	404	446	rVB	483199	1193472	3.35%	2.728%
3	3.043	539	545	548	rBV5	1707235	1715249	4.81%	3.921%
4	6.222	1516	1534	1552	rBV2	240617	552219	1.55%	1.262%
5	6.650	1654	1667	1686	rBV	277354	516686	1.45%	1.181%
6	8.103	2107	2119	2134	rBV	304926	542127	1.52%	1.239%
7	8.769	2310	2326	2342	rBV	172871	439747	1.23%	1.005%
8	9.518	2545	2559	2570	rBV	342439	598472	1.68%	1.368%
9	11.836	3268	3280	3297	rVB	354436	658033	1.85%	1.504%
10	12.213	3384	3397	3413	rVB	261404	475587	1.33%	1.087%
11	17.454	5015	5027	5054	rBV2	655128	1425831	4.00%	3.259%

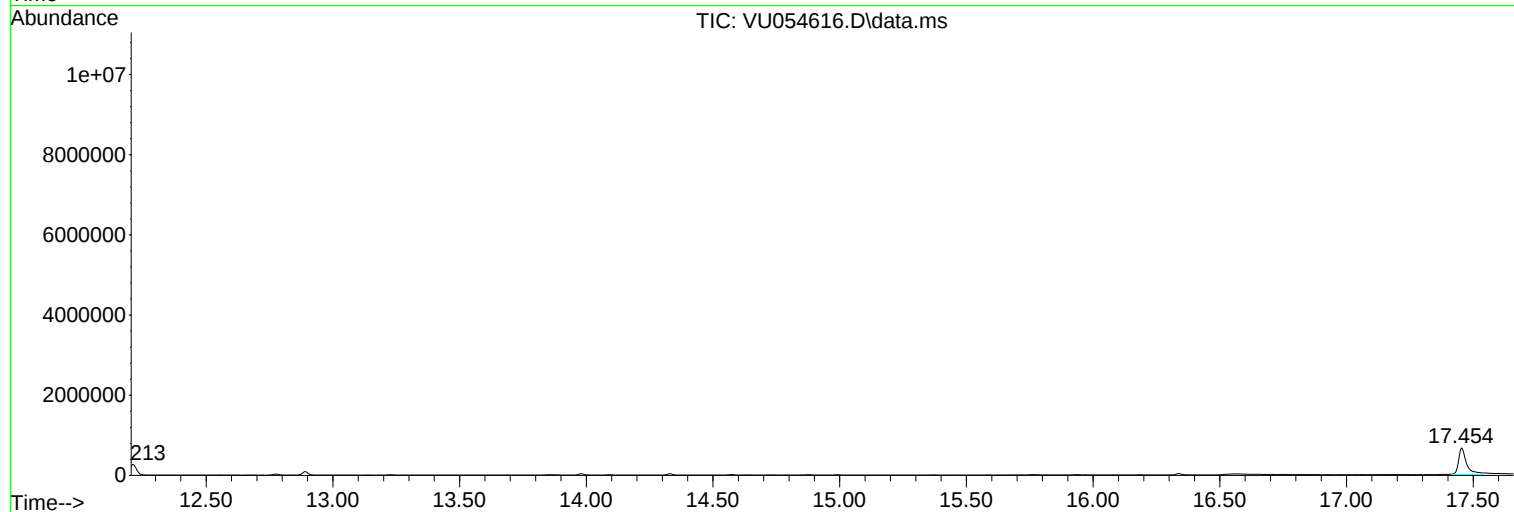
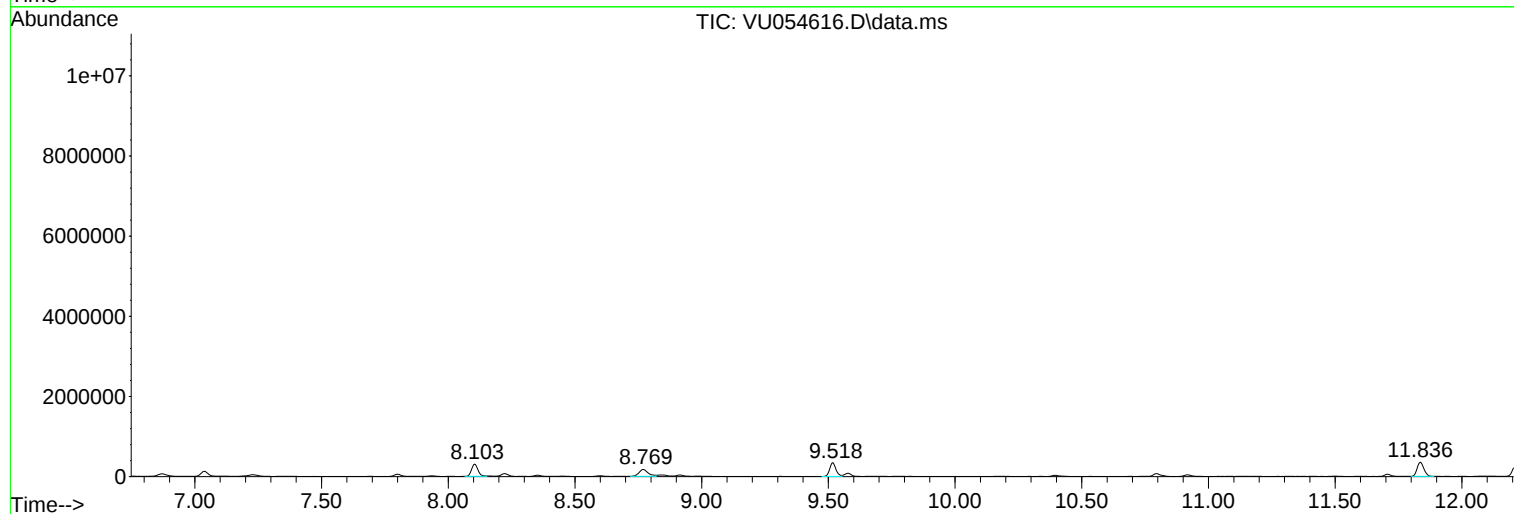
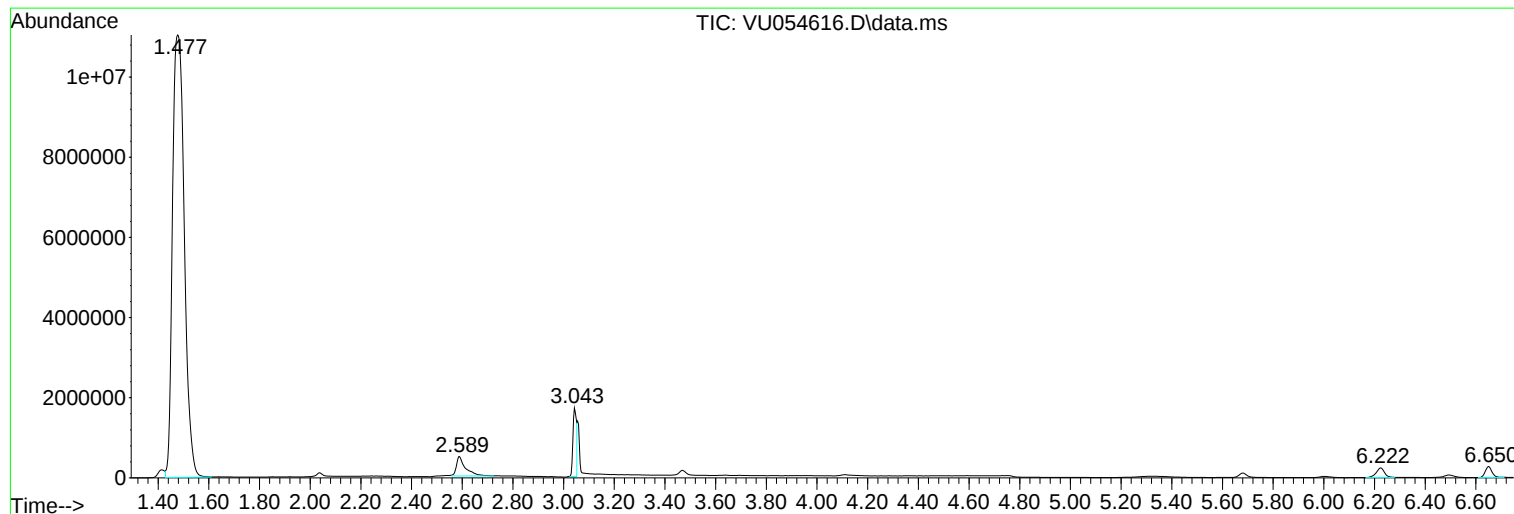
Sum of corrected areas: 43746864

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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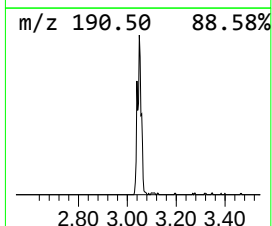
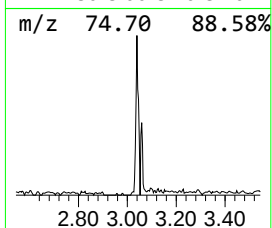
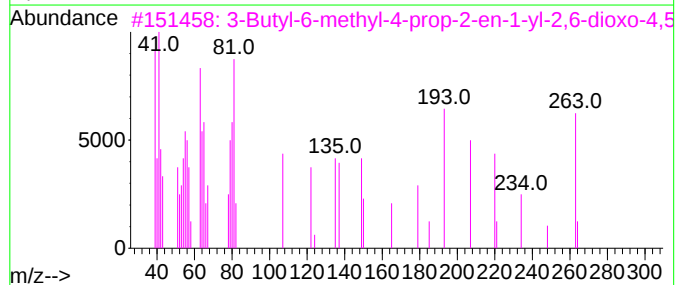
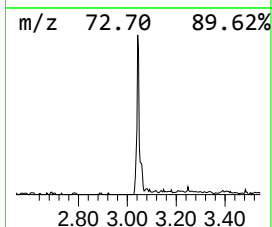
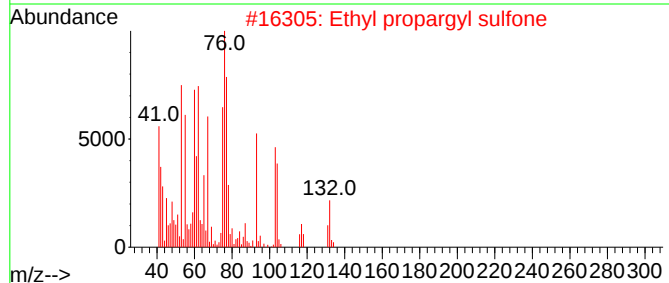
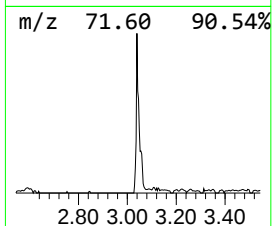
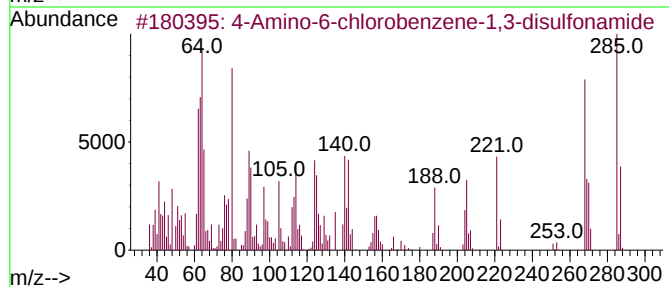
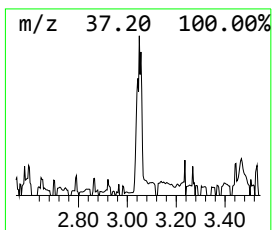
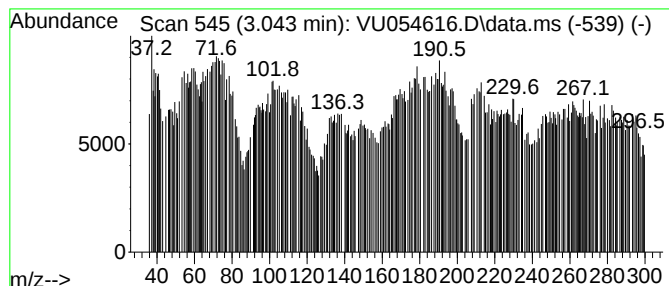
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 4-Amino-6-chlorobenzene-1,3... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.043	16.60 ug/L	1715250	1,4-Difluorobenzene	6.650	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-6-chlorobenzene-1,3-disu...	285	C6H8ClN3O4S2	000121-30-2	70
2	Ethyl propargyl sulfone	132	C5H8O2S	013603-87-7	68
3	3-Butyl-6-methyl-4-prop-2-en-1-y...	263	C12H17N5O2	1000312-01-1	55
4	2-Bromo-5-chloro-3-nitropyridine	236	C5H2BrClN2O2	075806-86-9	51
5	4,6-Diformyl-2,5-dimethoxytropone	222	C11H10O5	1000433-29-9	50



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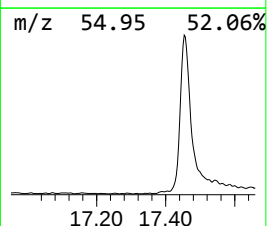
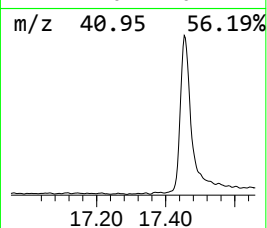
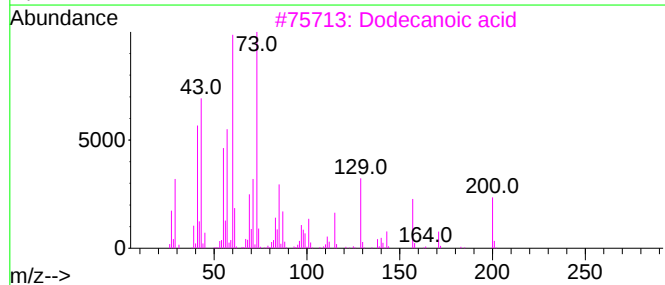
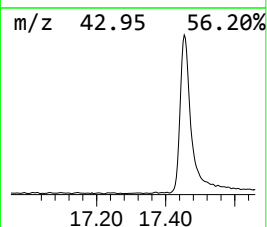
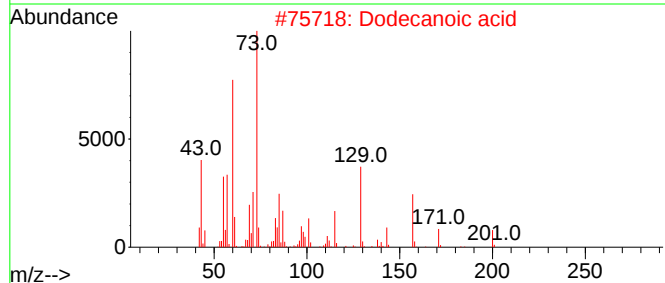
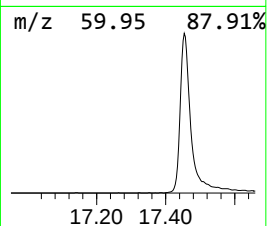
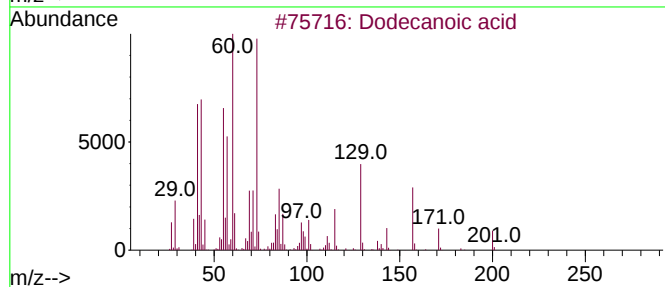
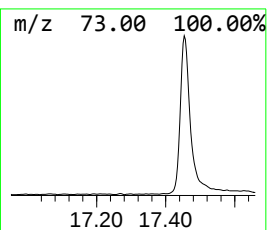
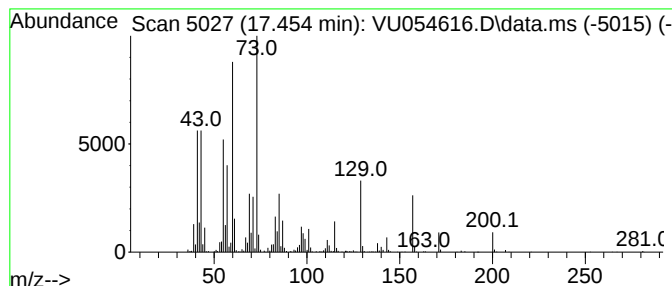
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Peak Number 3 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.453	10.83 ug/L	1425830	1,4-Dichlorobenzene-d4	11.836

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	99
2			Dodecanoic acid	200	C12H24O2	000143-07-7	98
3			Dodecanoic acid	200	C12H24O2	000143-07-7	93
4			Dodecanoic acid	200	C12H24O2	000143-07-7	93
5			Tridecanoic acid	214	C13H26O2	000638-53-9	80



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Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Amino-6-chlor...	3.043	16.6	ug/L	1715250	1	6.650	516686	5.0
Dodecanoic acid	17.453	10.8	ug/L	1425830	3	11.836	658033	5.0