

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122822\
 Data File : VU052593.D
 Acq On : 28 Dec 2022 17:28
 Operator : JC/MD
 Sample : VIBLK141
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VIBLK141

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\SFAMUTR122022WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU052593.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	73	80	93	rVB	73425	83925	8.21%	1.308%
2	1.912	171	178	198	rVB	74526	103451	10.12%	1.612%
3	2.565	370	381	395	rVB	128118	209014	20.45%	3.257%
4	4.671	1011	1036	1089	rBV2	53040	353376	34.58%	5.506%
5	5.060	1140	1157	1178	rBV	141561	320552	31.37%	4.995%
6	5.491	1278	1291	1292	rBV2	52658	104560	10.23%	1.629%
7	5.723	1348	1363	1379	rVB2	276395	697718	68.27%	10.872%
8	6.247	1516	1526	1540	rVB	227979	423884	41.48%	6.605%
9	6.687	1653	1663	1682	rVB	190612	376853	36.88%	5.872%
10	7.562	1927	1935	1950	rVB	85985	149982	14.68%	2.337%
11	7.893	2028	2038	2059	rVB	297501	518820	50.77%	8.084%
12	8.176	2119	2126	2139	rVB2	55999	92730	9.07%	1.445%
13	8.639	2258	2270	2309	rVB2	446553	1021939	100.00%	15.923%
14	9.414	2500	2511	2526	rVB	313946	517877	50.68%	8.069%
15	10.751	2916	2927	2943	rBV	163563	264924	25.92%	4.128%
16	11.806	3244	3255	3272	rBV	301769	473230	46.31%	7.374%
17	12.189	3363	3374	3389	rBV	305028	482756	47.24%	7.522%
18	17.452	5002	5011	5027	rBV2	126400	222227	21.75%	3.463%

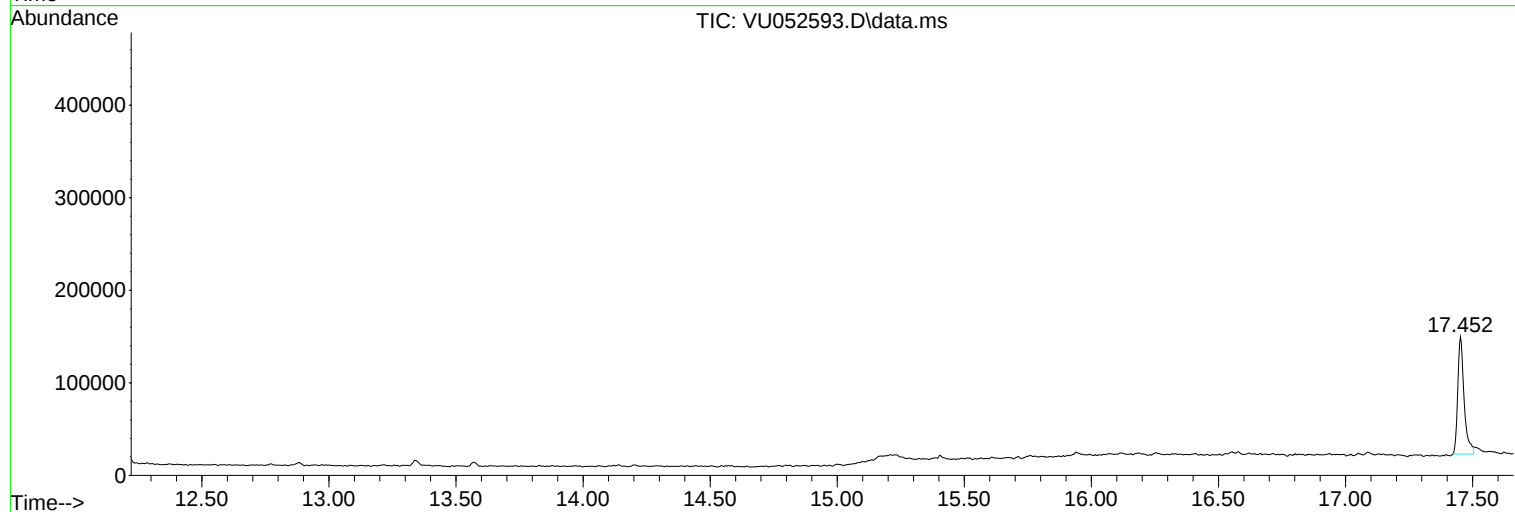
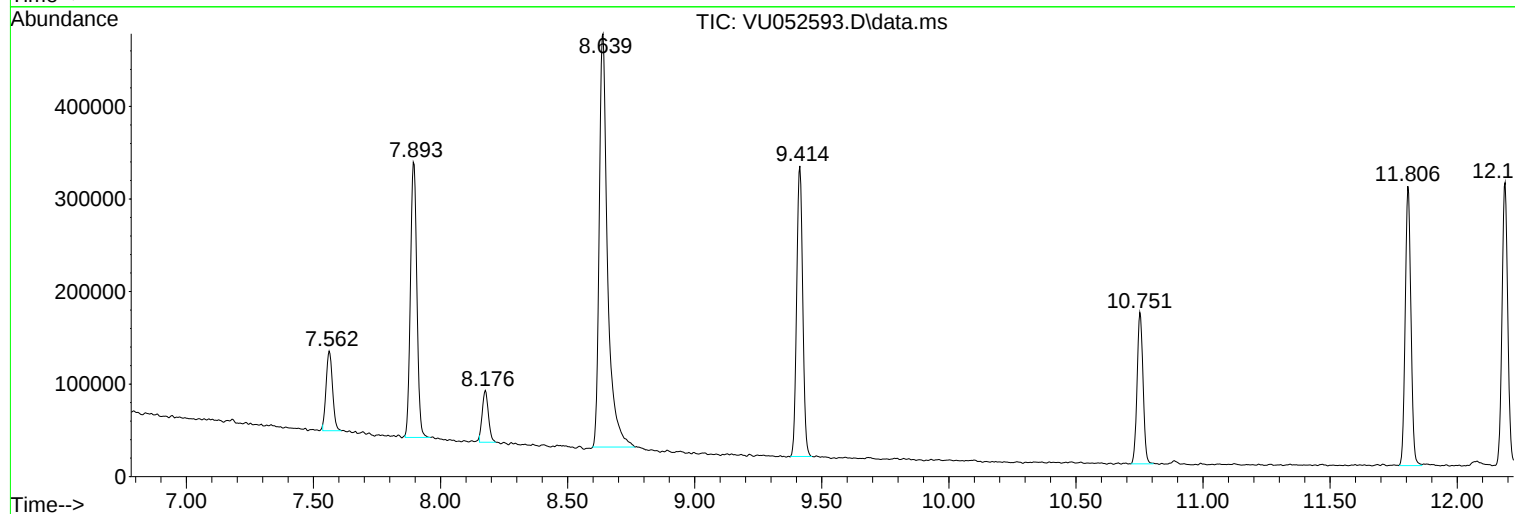
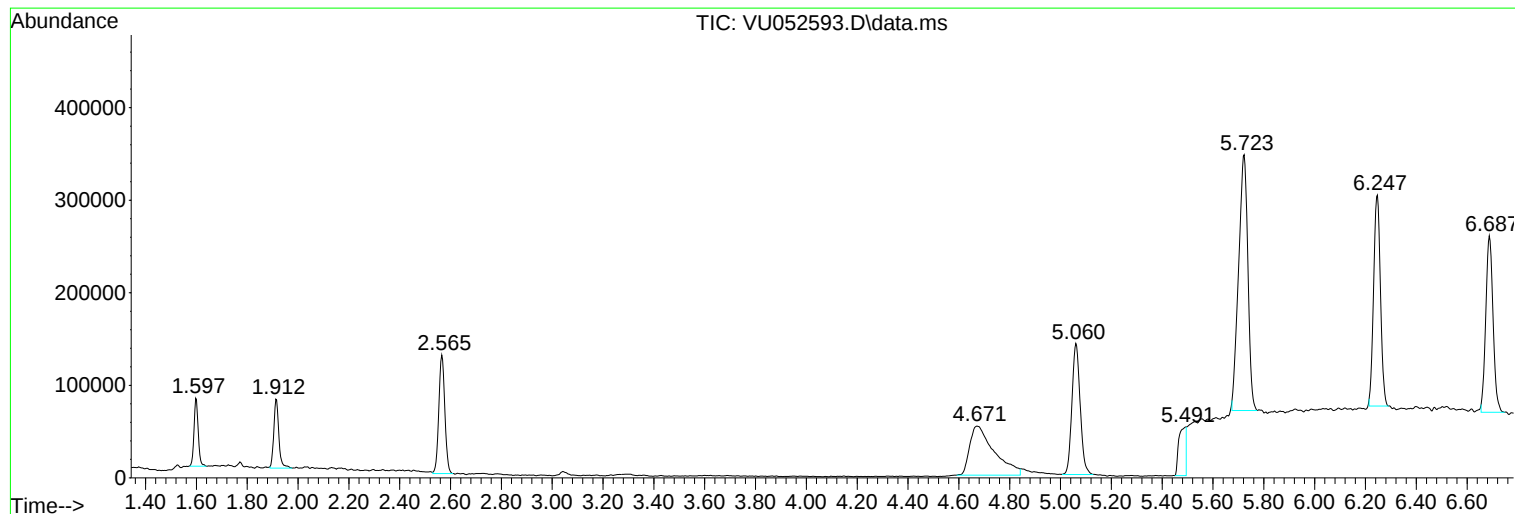
Sum of corrected areas: 6417818

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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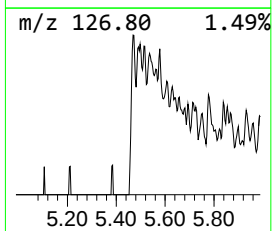
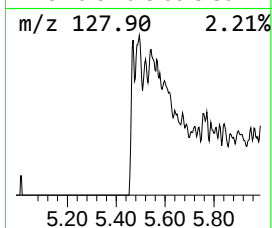
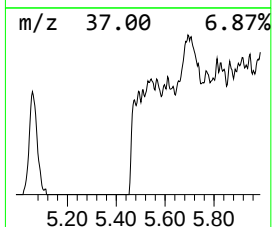
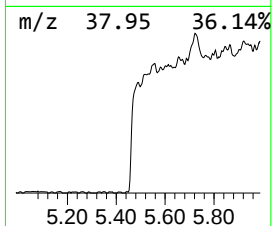
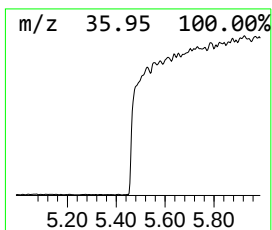
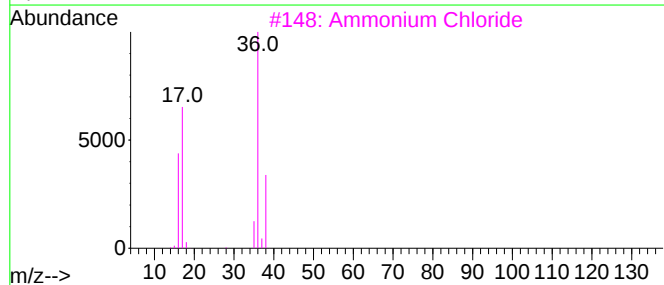
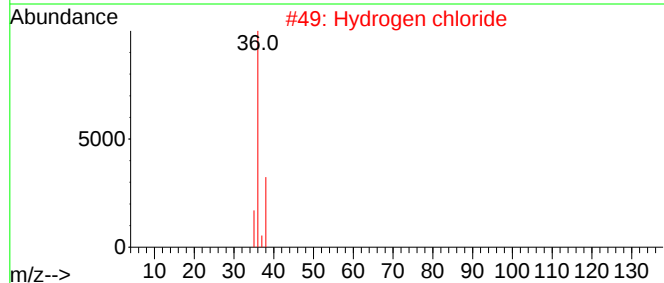
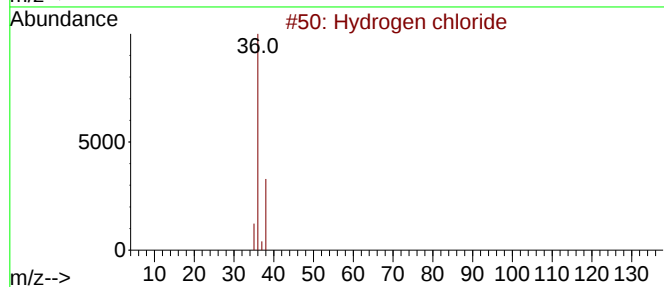
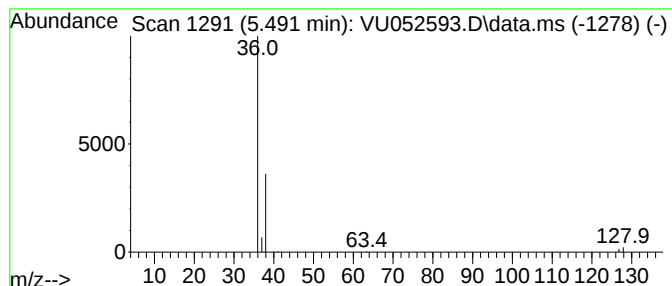
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122022WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.491	1.23 ug/L	104560	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hydrogen chloride	36	ClH	007647-01-0	9
2			Hydrogen chloride	36	ClH	007647-01-0	9
3			Ammonium Chloride	53	ClH4N	012125-02-9	4
4			Methanol-D4	36	CD4O	000811-98-3	2
5			1H-Imidazole-1-ethanol, .alpha.-...	126	C6H10N2O	037788-55-9	2



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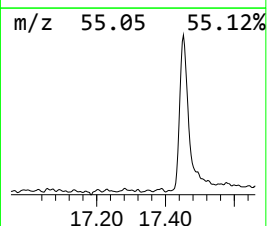
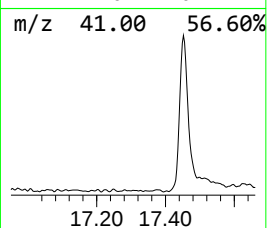
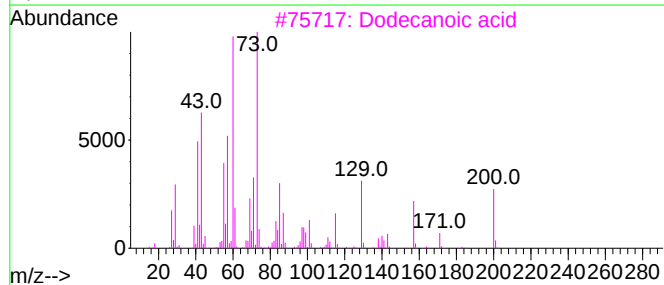
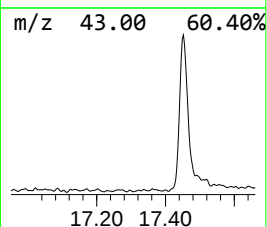
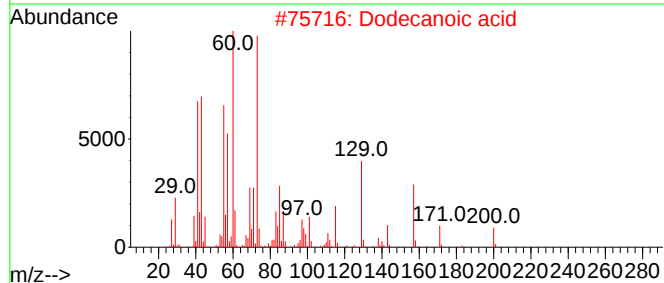
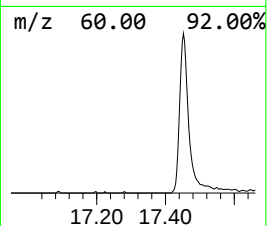
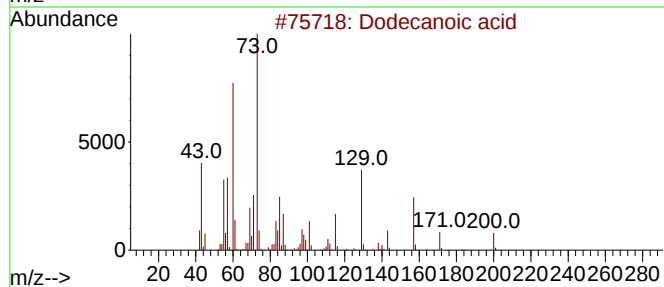
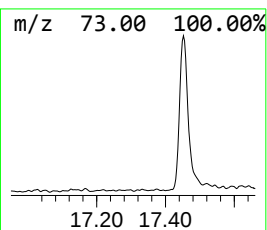
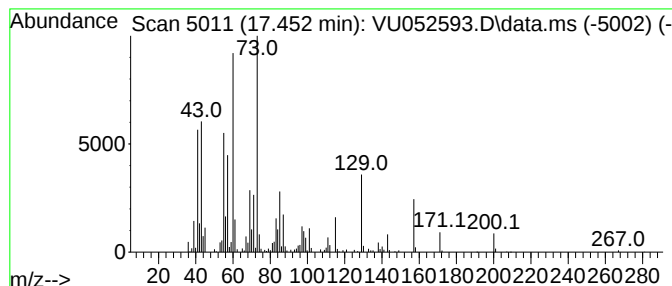
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.452	2.35 ug/L	222227	1,4-Dichlorobenzene-d4	11.806

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	98
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	91
5			Dodecanoic acid	200	C12H24O2	000143-07-7	87



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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
unknown-01	5.491	1.2	ug/L	104560	1	6.247	423884	5.0
Dodecanoic acid	17.452	2.4	ug/L	222227	3	11.806	473230	5.0