

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061923\
 Data File : VU054601.D
 Acq On : 19 Jun 2023 17:08
 Operator : MD/SY
 Sample : 03232-01DL 10X
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 CONK7DL

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: VU054601.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.599	89	96	110	rVB	58107	69412	4.16%	0.750%
2	1.911	185	193	206	rBV	81656	115083	6.90%	1.243%
3	2.563	384	396	409	rBV2	120101	202313	12.14%	2.186%
4	3.042	532	545	562	rVB2	14650	27834	1.67%	0.301%
5	3.866	790	801	816	rVB3	10254	25744	1.54%	0.278%
6	4.640	1027	1042	1084	rBV2	129110	497086	29.82%	5.371%
7	5.058	1156	1172	1195	rVB2	159563	359855	21.58%	3.888%
8	5.312	1232	1251	1271	rBV	733170	1667175	100.00%	18.013%
9	5.721	1357	1378	1400	rBV2	303295	810001	48.59%	8.752%
10	6.245	1527	1541	1566	rBV	294259	574253	34.44%	6.204%
11	6.541	1621	1633	1651	rBV3	39635	76877	4.61%	0.831%
12	6.685	1663	1678	1695	rBV	210456	419191	25.14%	4.529%
13	7.563	1937	1951	1970	rBV	82813	152895	9.17%	1.652%
14	7.894	2038	2054	2069	rBV	329934	572247	34.32%	6.183%
15	8.177	2128	2142	2155	rBV2	52848	94440	5.66%	1.020%
16	8.470	2222	2233	2244	rBV	18394	34620	2.08%	0.374%
17	8.631	2271	2283	2315	rBV	523044	1062644	63.74%	11.481%
18	9.412	2515	2526	2544	rBV	408627	690398	41.41%	7.459%
19	10.753	2931	2943	2958	rBV2	179250	284353	17.06%	3.072%
20	10.888	2976	2985	3000	rVB	26796	45895	2.75%	0.496%
21	11.807	3259	3271	3290	rBV	415122	672650	40.35%	7.268%
22	12.190	3377	3390	3406	rBV	343677	569083	34.13%	6.149%
23	16.338	4672	4680	4691	rVB4	24584	34896	2.09%	0.377%
24	17.457	5019	5028	5049	rBV2	94054	196522	11.79%	2.123%

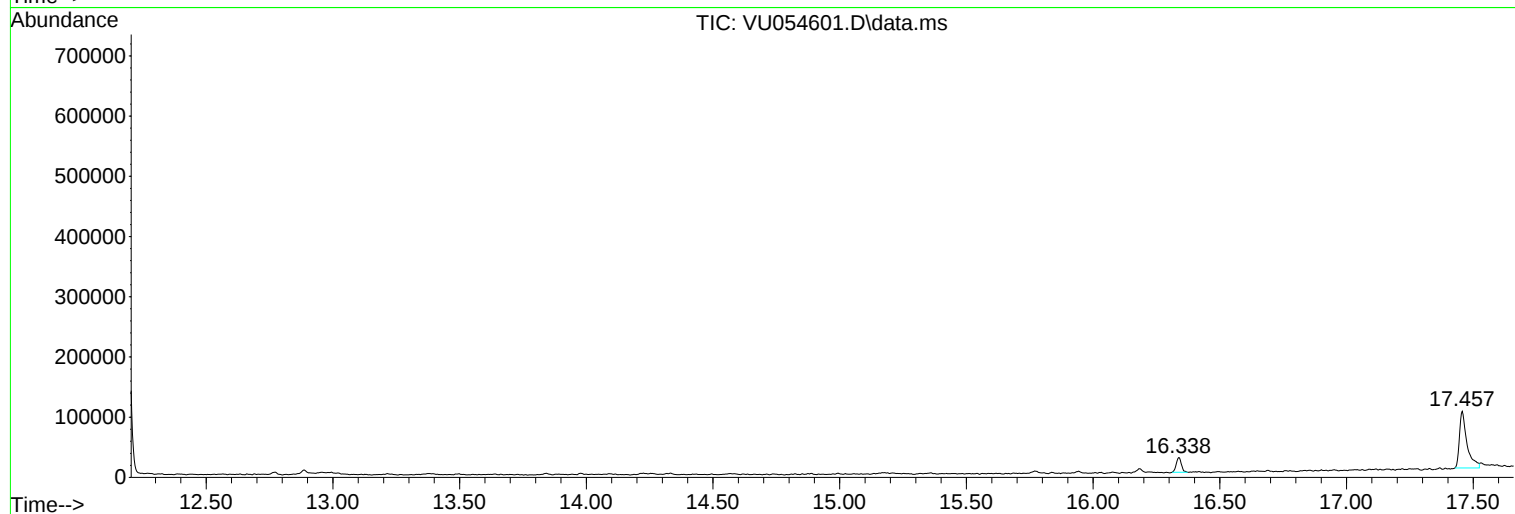
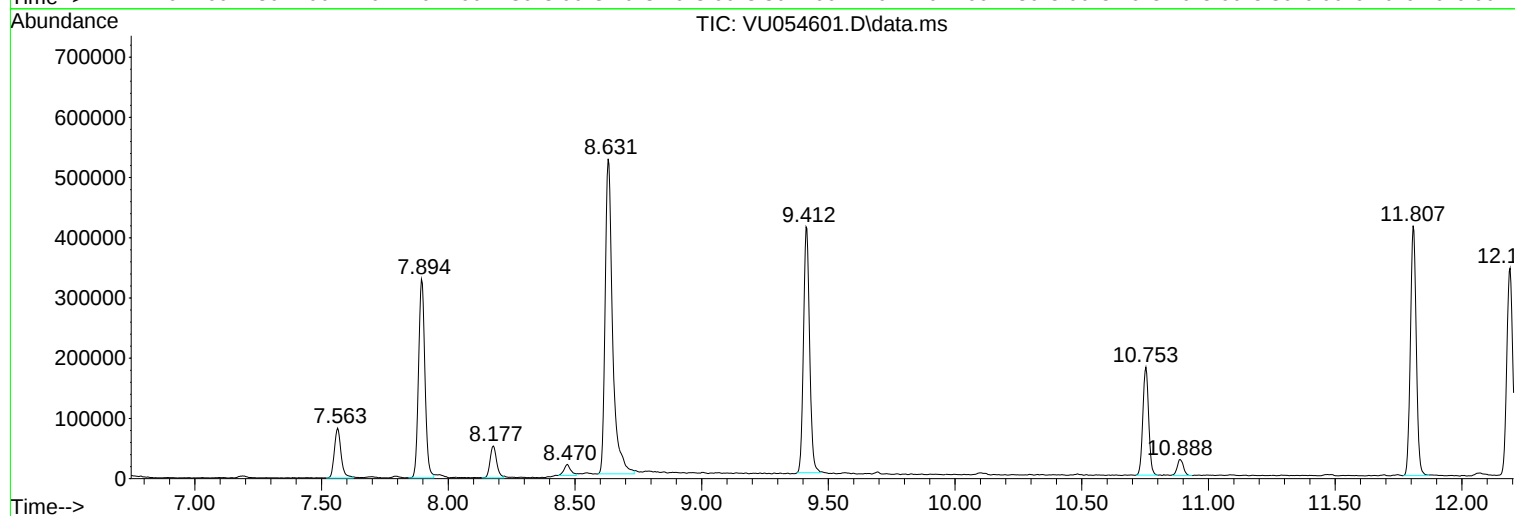
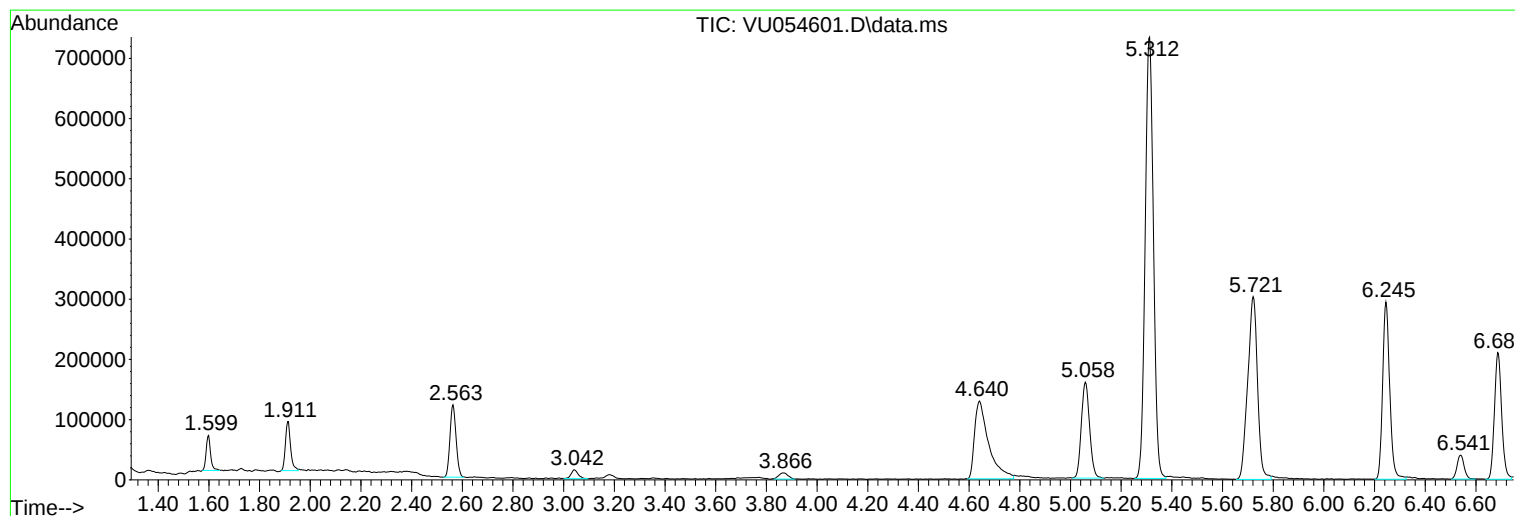
Sum of corrected areas: 9255467

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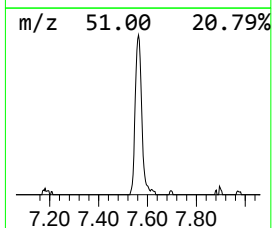
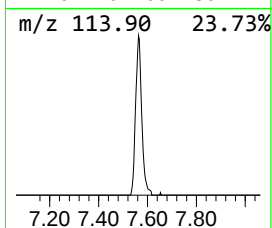
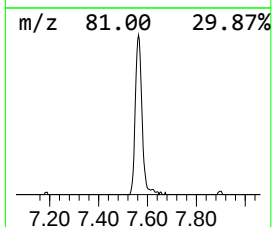
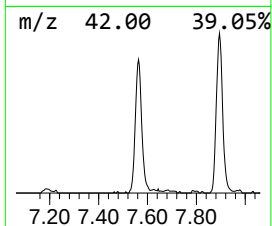
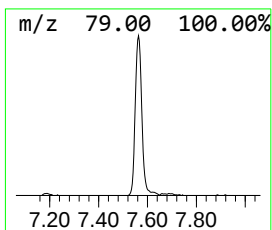
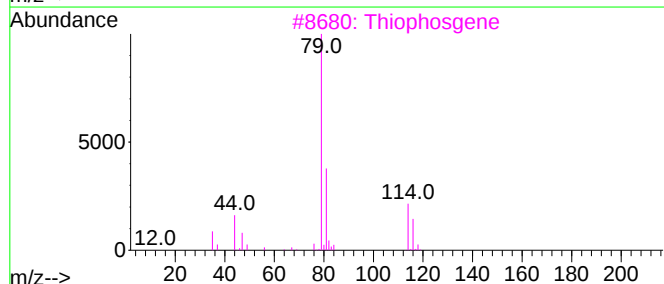
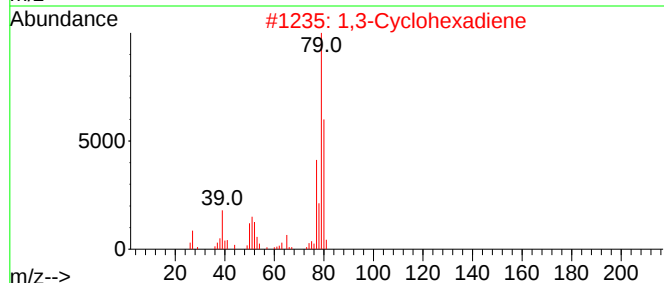
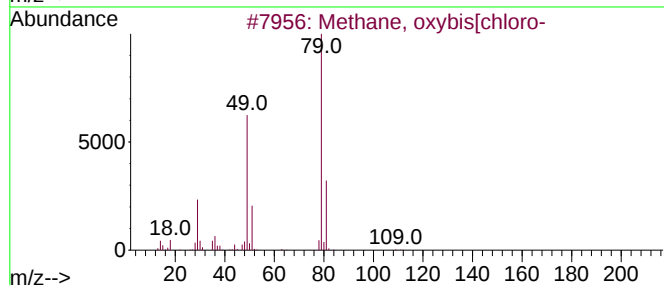
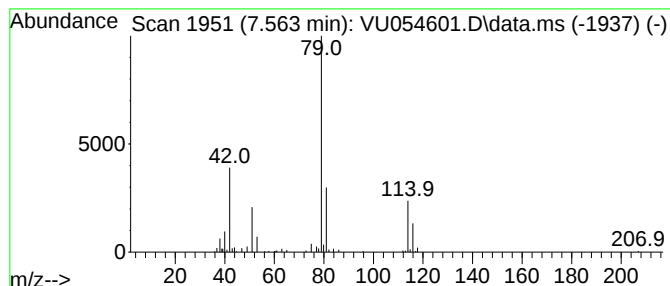
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR060723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.563	1.33 ug/L	152895	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, oxybis[chloro-	114	C2H4Cl2O	000542-88-1	37
2			1,3-Cyclohexadiene	80	C6H8	000592-57-4	37
3			Thiophosgene	114	CCl2S	000463-71-8	28
4			2-Propanol, 1,3-dichloro-	128	C3H6Cl2O	000096-23-1	23
5			3-Thiatricyclo[3.1.1.0(2,4)]heptane	112	C6H8S	1000221-37-0	9



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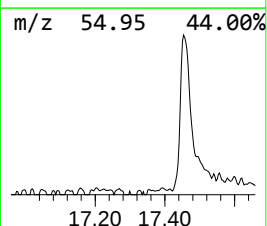
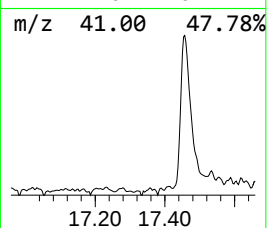
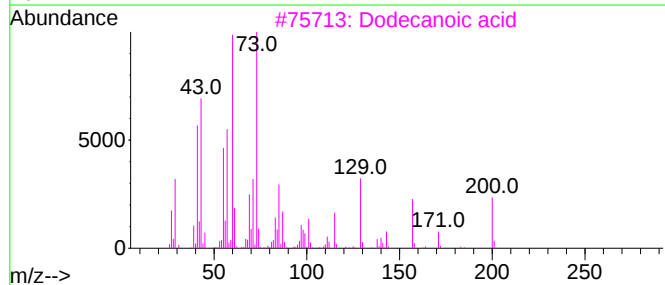
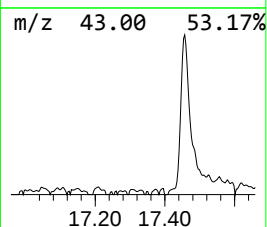
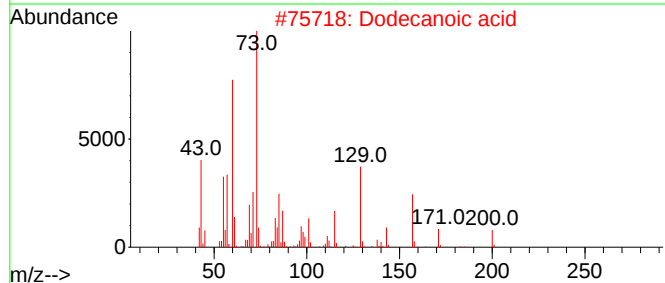
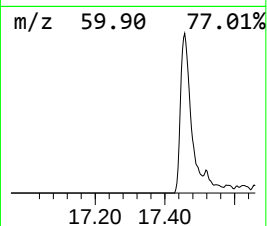
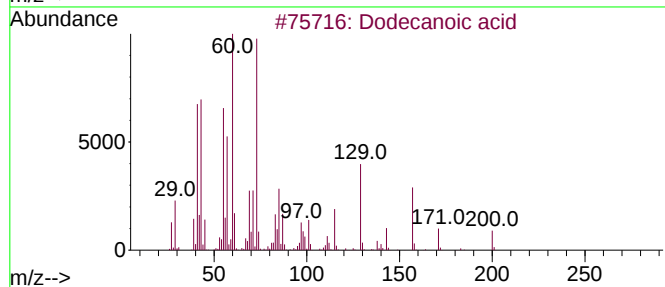
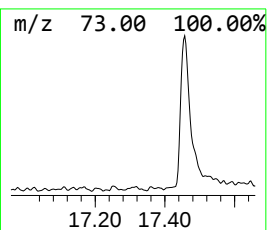
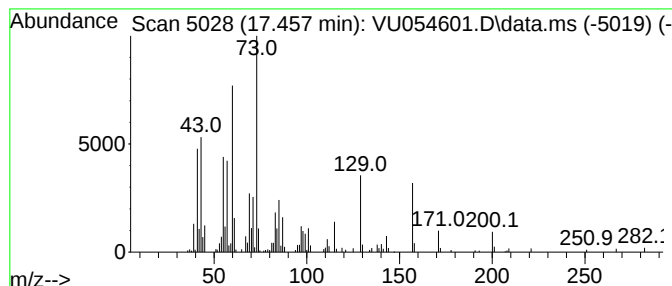
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Dodecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.457	1.46 ug/L	196522	1,4-Dichlorobenzene-d4	11.807

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	96
4			Dodecanoic acid	200	C12H24O2	000143-07-7	93
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	68



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C0NK7DL

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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
unknown-01	7.563	1.3	ug/L	152895	1	6.245	574253	5.0
Dodecanoic acid	17.457	1.5	ug/L	196522	3	11.807	672650	5.0