

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122823\
 Data File : VU057352.D
 Acq On : 28 Dec 2023 22:48
 Operator : MD/SY
 Sample : 06020-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH7Y1

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\SFAMUTR122723WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057352.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.309	3	6	19	rVB	641721	800214	97.99%	9.955%
2	1.364	19	23	34	rVB	19345	27723	3.39%	0.345%
3	1.486	54	61	69	rBV	34739	44102	5.40%	0.549%
4	1.531	69	75	82	rVV	23789	30297	3.71%	0.377%
5	1.576	83	89	100	rVB	21457	29012	3.55%	0.361%
6	1.644	104	110	124	rVB	19708	30193	3.70%	0.376%
7	1.718	126	133	138	rBV	12883	19196	2.35%	0.239%
8	1.766	139	148	168	rVB2	105521	196581	24.07%	2.445%
9	2.190	271	280	300	rBV	91312	162454	19.89%	2.021%
10	3.039	533	544	559	rVB	140515	253256	31.01%	3.151%
11	5.515	1301	1314	1347	rBV	223215	483151	59.16%	6.010%
12	6.078	1470	1489	1509	rBV2	359292	816624	100.00%	10.159%
13	6.531	1617	1630	1647	rBV	280111	521294	63.84%	6.485%
14	6.766	1692	1703	1724	rVB7	12813	39519	4.84%	0.492%
15	6.933	1737	1755	1775	rBV	196219	386862	47.37%	4.813%
16	7.132	1802	1817	1833	rVB6	18964	54792	6.71%	0.682%
17	7.727	1987	2002	2016	rBV2	76231	139041	17.03%	1.730%
18	7.865	2032	2045	2062	rVB4	6401	14563	1.78%	0.181%
19	8.039	2085	2099	2113	rBV	320376	578304	70.82%	7.194%
20	8.110	2114	2121	2125	rBV2	17432	24720	3.03%	0.308%
21	8.299	2170	2180	2192	rBV	42504	74899	9.17%	0.932%
22	8.560	2249	2261	2274	rBV	52685	98556	12.07%	1.226%
23	8.634	2274	2284	2295	rVB5	6361	11868	1.45%	0.148%
24	8.737	2297	2316	2329	rBV	233450	539832	66.11%	6.716%
25	8.804	2331	2337	2357	rVB	64614	147294	18.04%	1.832%
26	9.486	2536	2549	2560	rBV	363092	628444	76.96%	7.818%
27	9.750	2621	2631	2640	rBV3	9662	17138	2.10%	0.213%
28	10.782	2938	2952	2971	rBV	109050	216568	26.52%	2.694%
29	10.907	2980	2991	3008	rBV2	53582	98081	12.01%	1.220%
30	11.827	3264	3277	3294	rBV	311087	560400	68.62%	6.971%
31	12.074	3344	3354	3382	rBV6	19593	80380	9.84%	1.000%
32	12.203	3382	3394	3416	rVB	309605	554262	67.87%	6.895%
33	12.772	3562	3571	3581	rVB	21636	34449	4.22%	0.429%
34	12.888	3598	3607	3619	rVB10	8389	14115	1.73%	0.176%
35	16.868	4836	4845	4856	rBV10	4574	10596	1.30%	0.132%
36	17.457	5017	5028	5054	rBV3	121581	299796	36.71%	3.729%

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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\SFAMUTR122723WMA.M
Title : TRACE VOA SFAM1.0

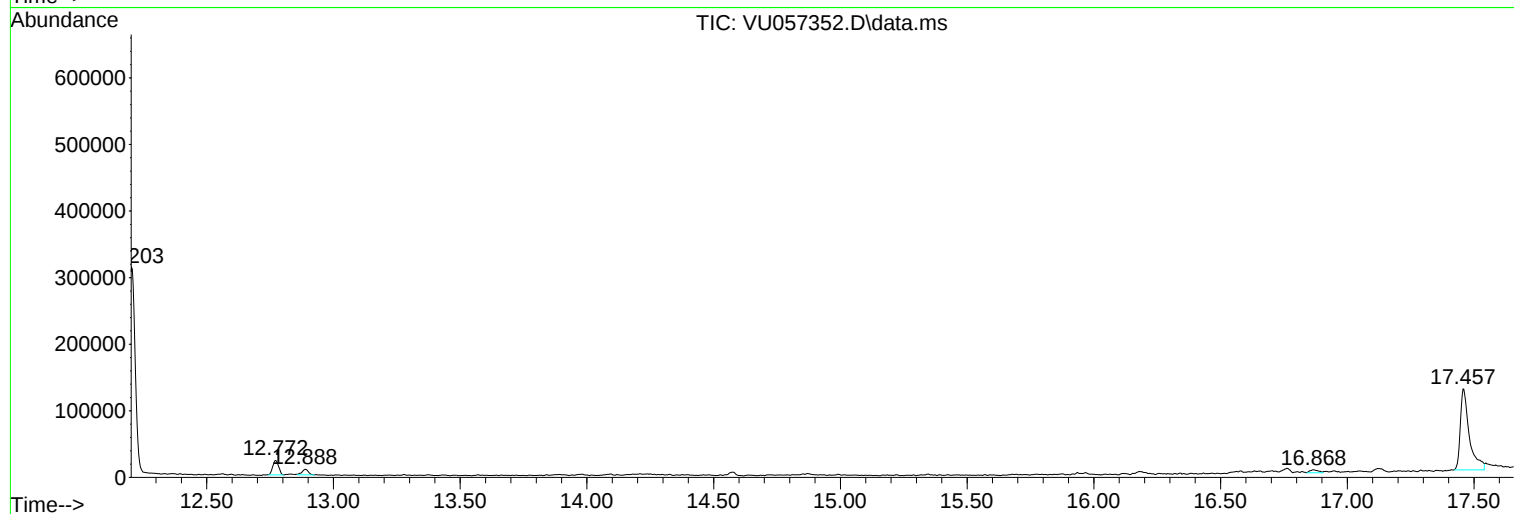
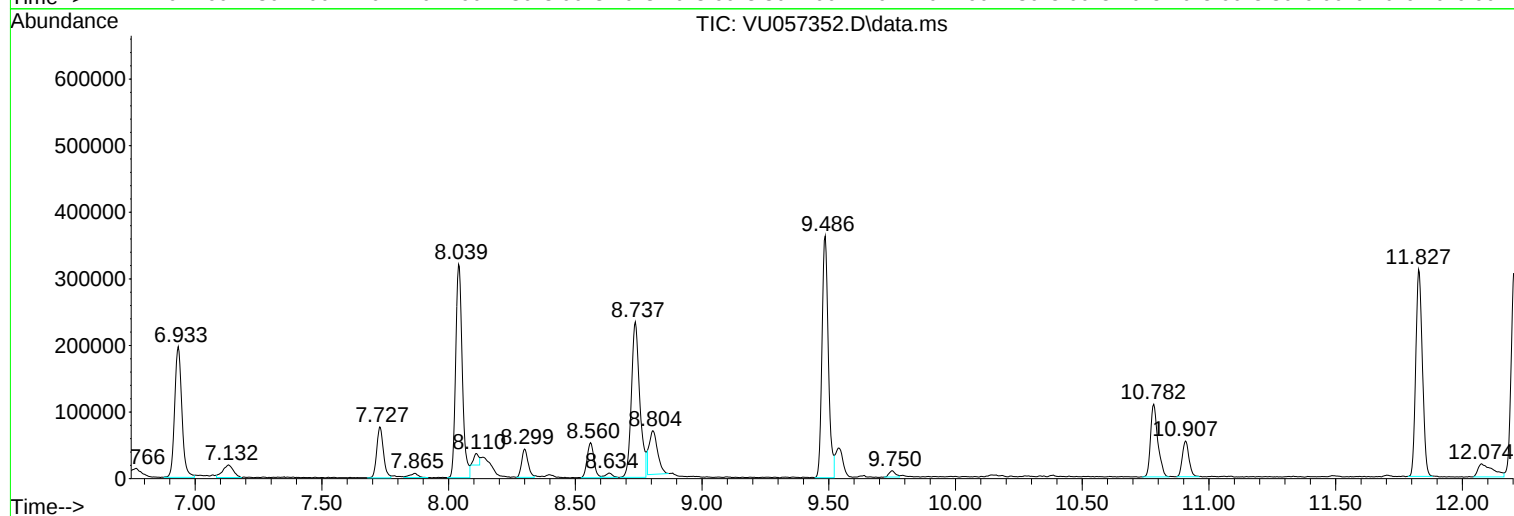
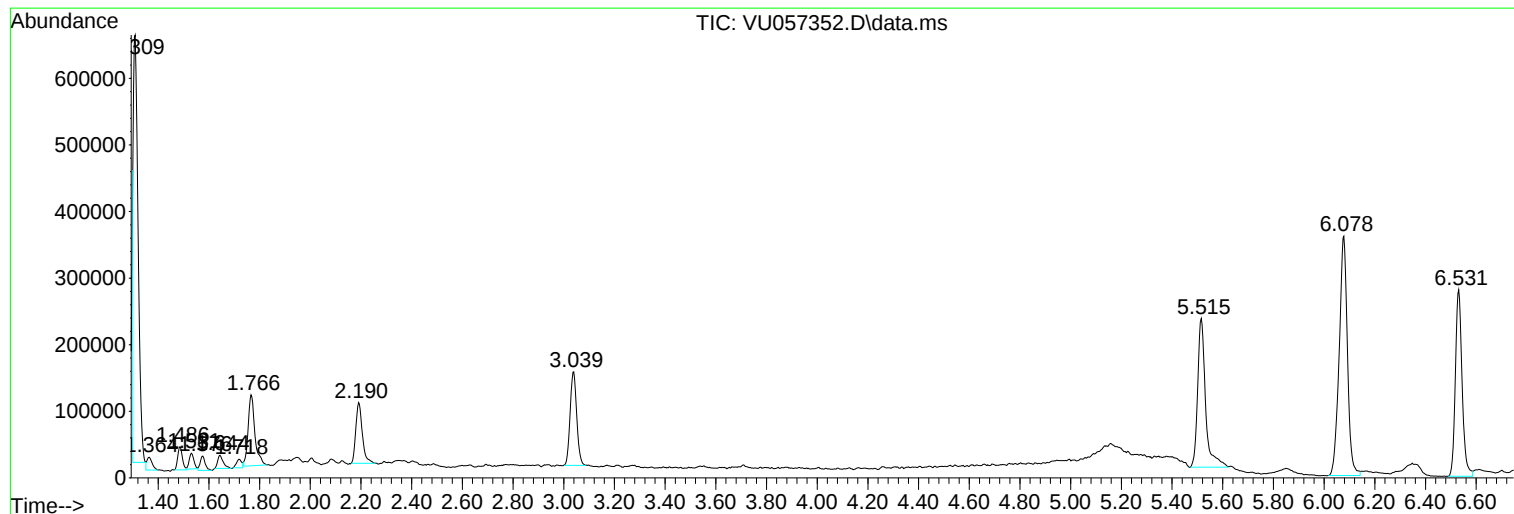
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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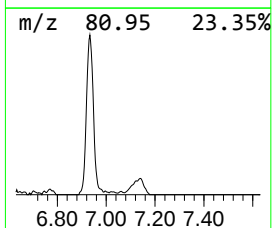
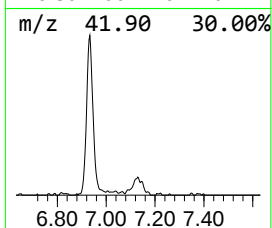
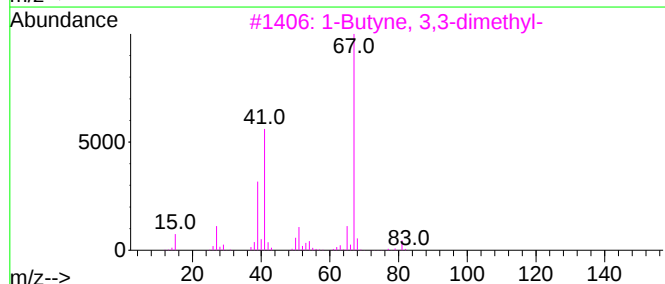
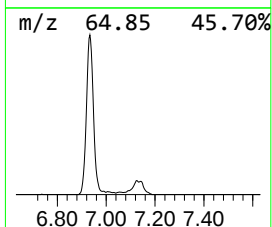
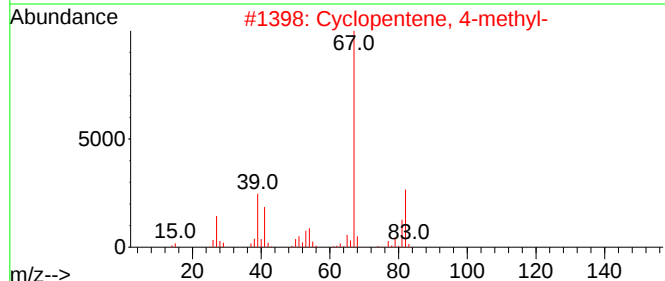
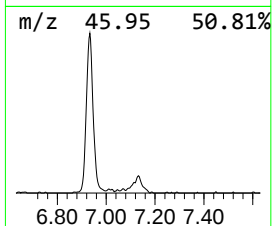
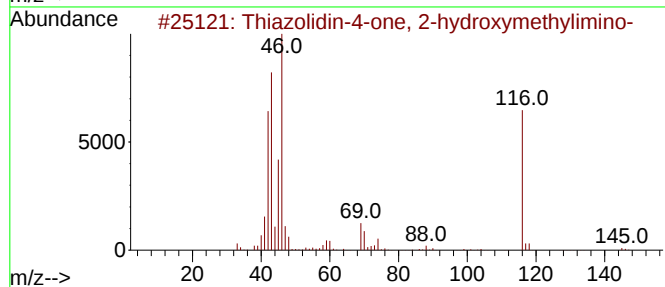
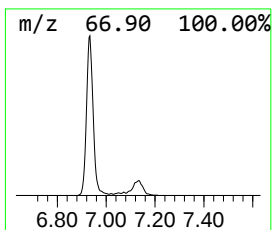
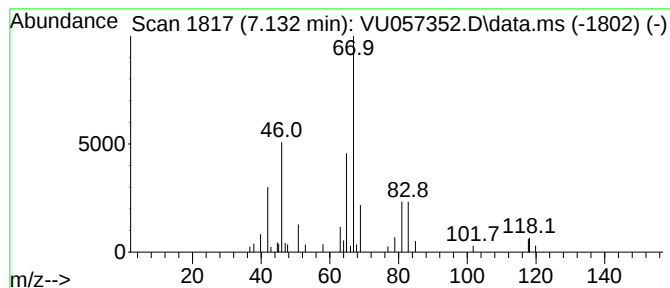
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.132	0.53 ug/L	54792	1,4-Difluorobenzene	6.531

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thiazolidin-4-one, 2-hydroxymeth...	146	C4H6N2O2S	104959-22-0	9
2			Cyclopentene, 4-methyl-	82	C6H10	001759-81-5	9
3			1-Butyne, 3,3-dimethyl-	82	C6H10	000917-92-0	9
4			Fluorodichloromethane	102	CHCl2F	000075-43-4	7
5			Cyclohexane, fluoro-	102	C6H11F	000372-46-3	5



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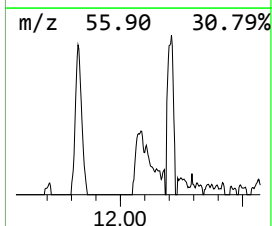
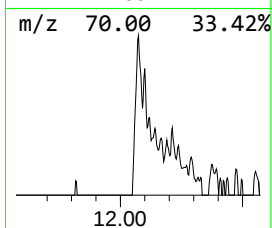
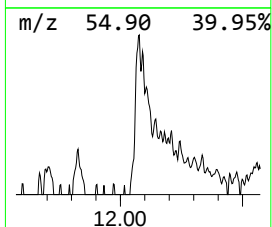
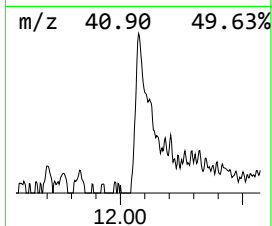
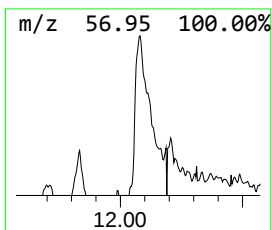
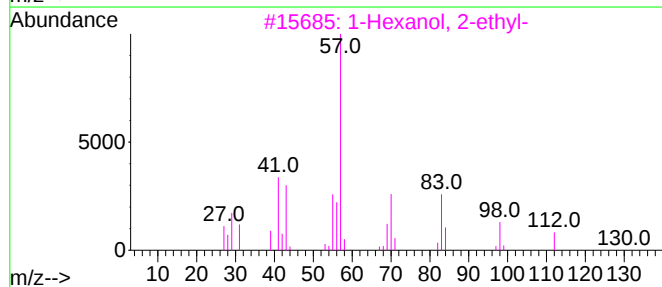
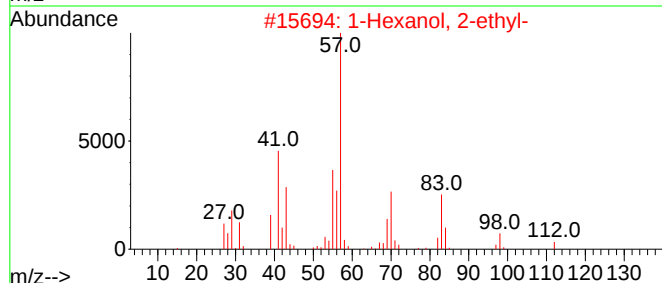
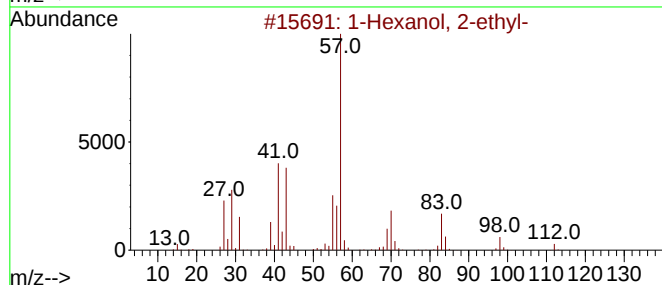
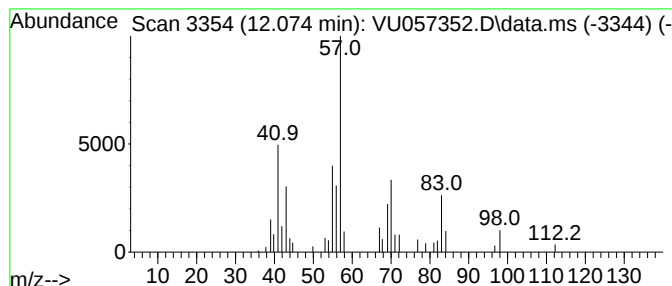
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.074	0.72 ug/L	80380	1,4-Dichlorobenzene-d4	11.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	59
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	56



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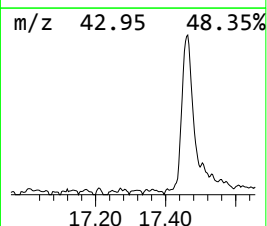
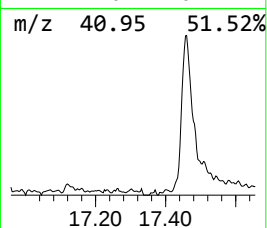
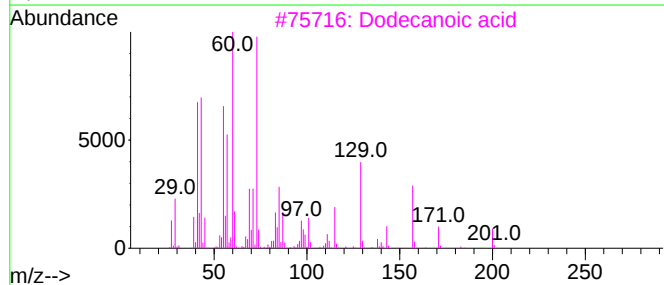
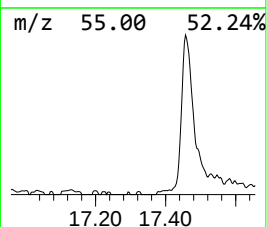
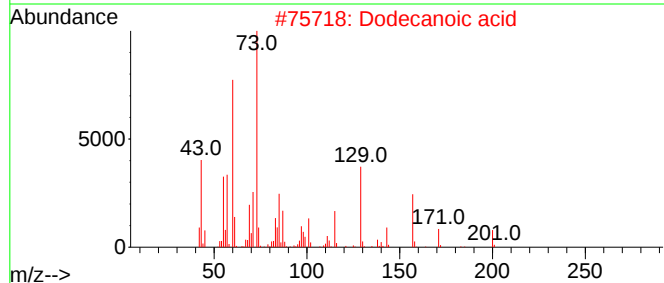
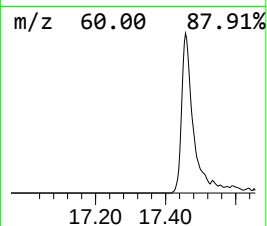
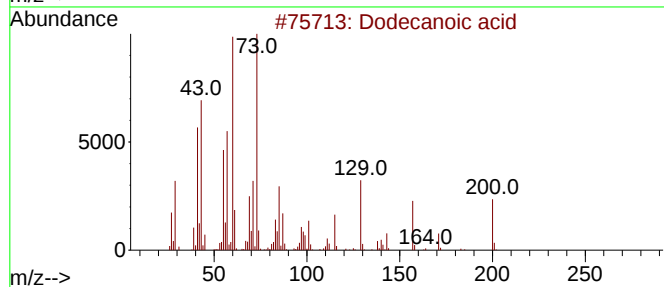
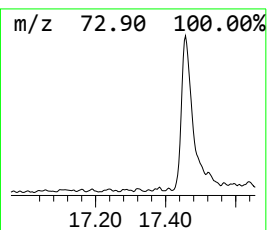
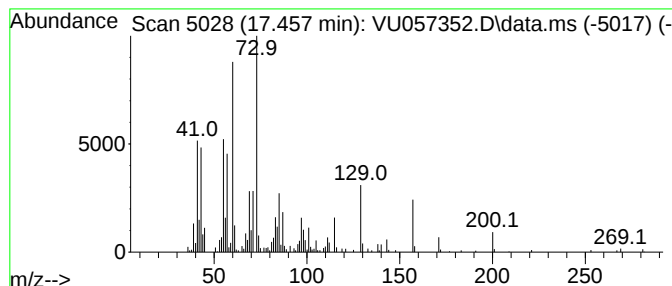
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122723WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.457	2.67 ug/L	299796	1,4-Dichlorobenzene-d4	11.827

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	96
2			Dodecanoic acid	200	C12H24O2	000143-07-7	94
3			Dodecanoic acid	200	C12H24O2	000143-07-7	93
4			Nonanoic acid	158	C9H18O2	000112-05-0	62
5			Dodecanoic acid	200	C12H24O2	000143-07-7	62



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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	7.132	0.5	ug/L	54792	1	6.531	521294	5.0
1-Hexanol, 2-et...	12.074	0.7	ug/L	80380	3	11.827	560400	5.0
Dodecanoic acid	17.457	2.7	ug/L	299796	3	11.827	560400	5.0