

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121623\
 Data File : VU056947.D
 Acq On : 17 Dec 2023 01:27
 Operator : MD/SY
 Sample : 05811-05
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 34 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F7B39

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\SFAMUTR121123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU056947.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	16	21	34	rVB2	17410	20663	2.33%	0.256%
2	1.486	50	61	67	rBV2	87273	164662	18.54%	2.037%
3	1.595	88	95	105	rVB2	129545	159682	17.98%	1.975%
4	1.727	129	136	147	rVB	55658	71814	8.09%	0.888%
5	1.911	185	193	209	rVV	82497	110950	12.49%	1.372%
6	1.991	212	218	226	rVB2	20064	27028	3.04%	0.334%
7	2.563	384	396	411	rBV2	165108	274838	30.95%	3.399%
8	2.679	423	432	442	rVB4	5308	9884	1.11%	0.122%
9	3.039	536	544	554	rBV8	4783	9622	1.08%	0.119%
10	3.132	562	573	581	rBV3	12256	22946	2.58%	0.284%
11	3.187	583	590	604	rVB3	5195	10924	1.23%	0.135%
12	3.354	632	642	655	rVB6	5213	10036	1.13%	0.124%
13	4.656	1023	1047	1076	rBV2	175363	658949	74.20%	8.151%
14	5.055	1156	1171	1189	rBV2	149783	338185	38.08%	4.183%
15	5.721	1357	1378	1406	rBV2	269534	728122	81.99%	9.006%
16	5.891	1417	1431	1447	rVB2	14955	34765	3.91%	0.430%
17	6.245	1528	1541	1563	rBV	237060	454880	51.22%	5.626%
18	6.537	1611	1632	1654	rBV	271625	524996	59.12%	6.494%
19	6.685	1664	1678	1699	rBV	200731	398028	44.82%	4.923%
20	7.251	1842	1854	1867	rVB4	17221	34553	3.89%	0.427%
21	7.377	1878	1893	1911	rVB2	27770	55371	6.24%	0.685%
22	7.563	1939	1951	1966	rBV	90025	162690	18.32%	2.012%
23	7.640	1966	1975	1987	rVB6	5124	10681	1.20%	0.132%
24	7.894	2041	2054	2070	rBV	329035	593739	66.86%	7.344%
25	8.177	2131	2142	2163	rBV2	51829	97473	10.98%	1.206%
26	8.470	2223	2233	2244	rBV	13843	23944	2.70%	0.296%
27	8.634	2272	2284	2319	rBV	435845	888056	100.00%	10.984%
28	8.904	2358	2368	2376	rBV3	8068	13487	1.52%	0.167%
29	9.338	2490	2503	2514	rBV	23487	41966	4.73%	0.519%
30	9.415	2515	2527	2555	rVV	372942	651258	73.34%	8.055%
31	9.695	2606	2614	2626	rVB6	5366	9045	1.02%	0.112%
32	10.753	2932	2943	2958	rBV	155455	250448	28.20%	3.098%
33	10.888	2974	2985	2996	rBV3	24112	39733	4.47%	0.491%
34	11.811	3259	3272	3288	rBV	348753	587636	66.17%	7.269%
35	12.065	3341	3351	3361	rBV5	13656	26762	3.01%	0.331%
36	12.190	3378	3390	3412	rBV	330598	566854	63.83%	7.011%

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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\SFAMUTR121123WMA.M
Title : TRACE VOA SFAM1.0

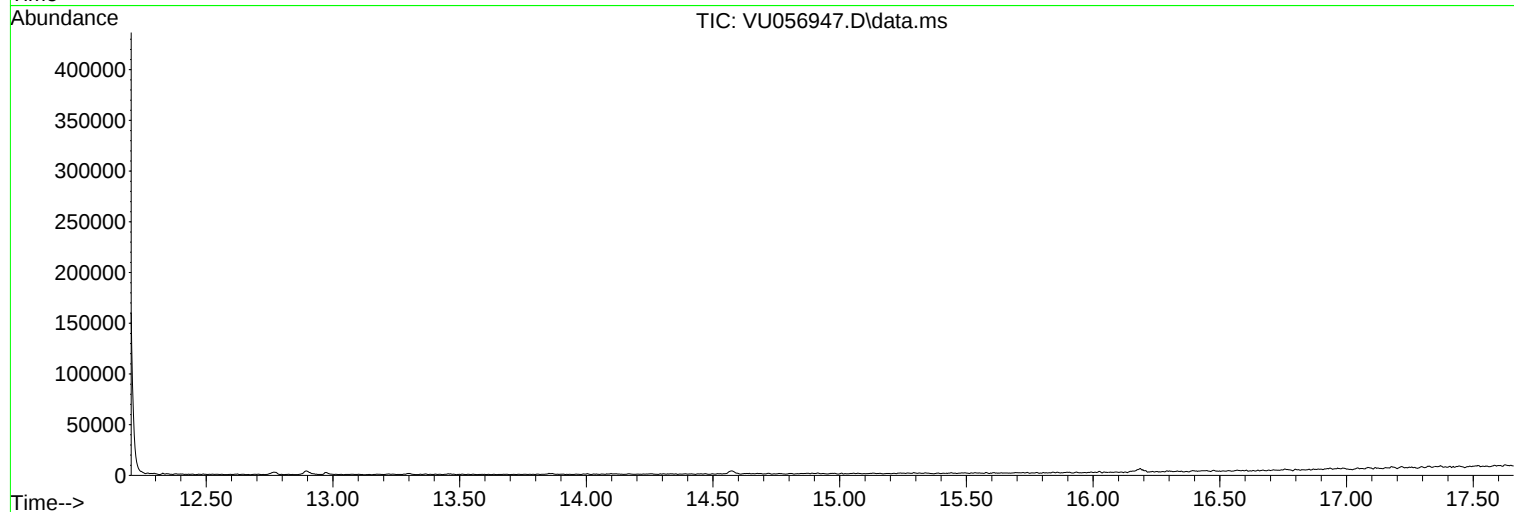
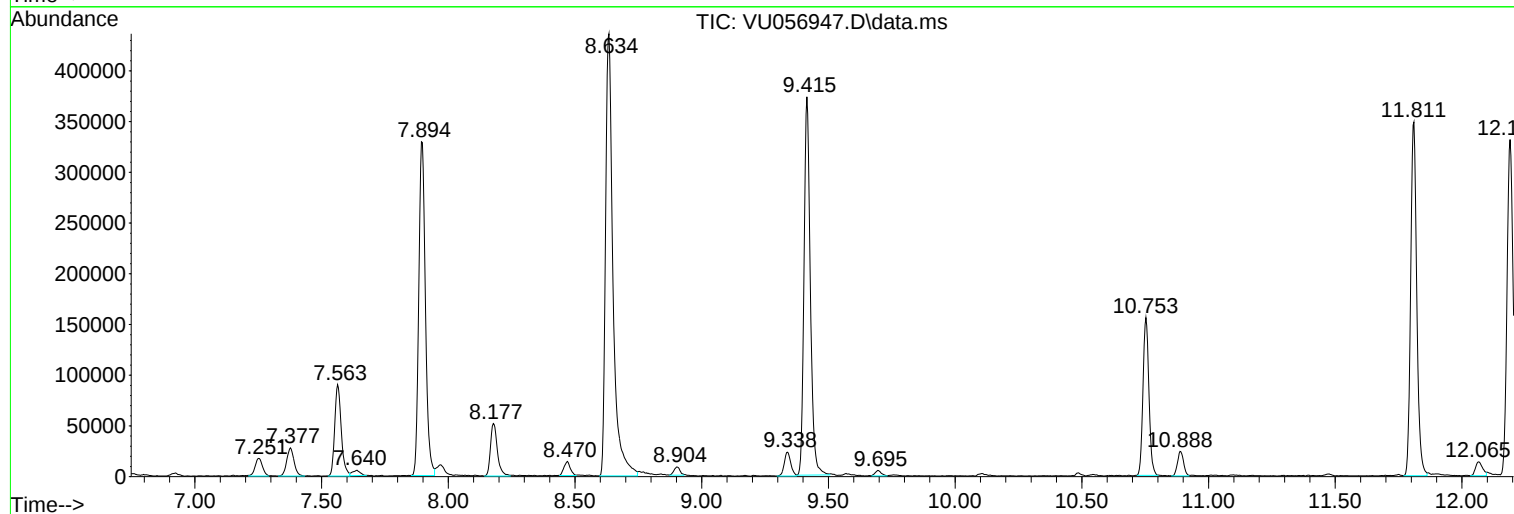
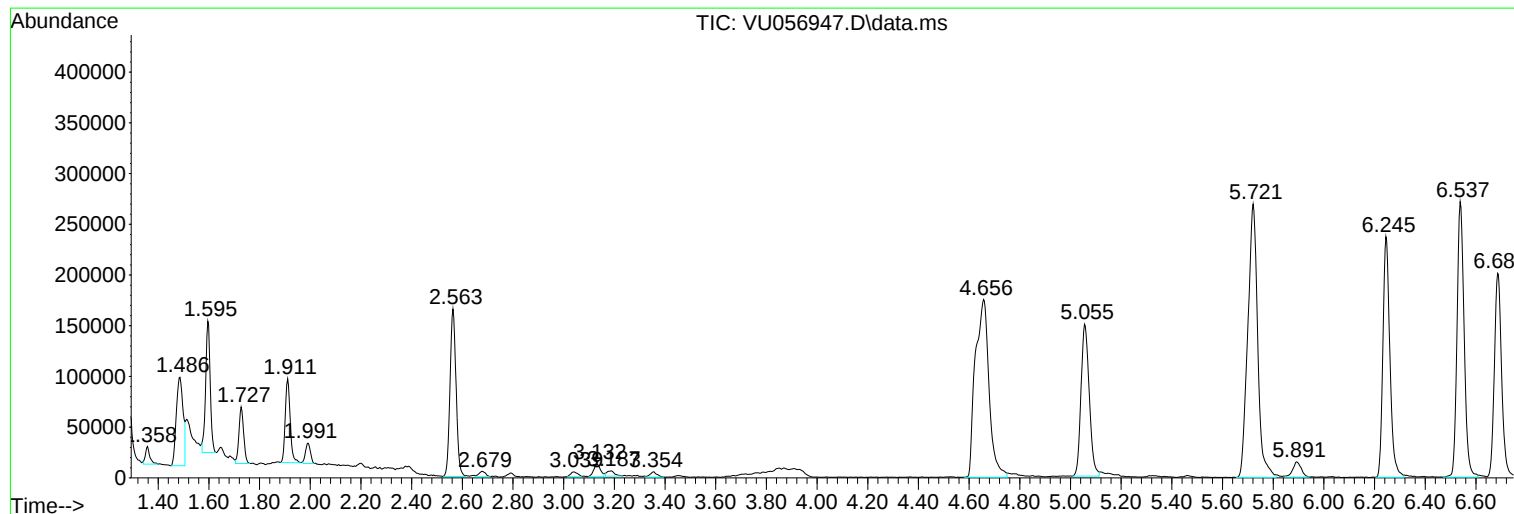
Sum of corrected areas: 8084670

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR121123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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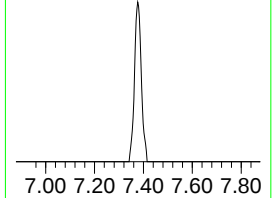
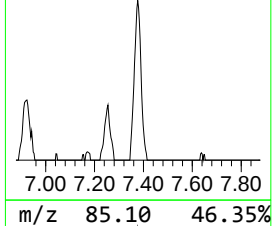
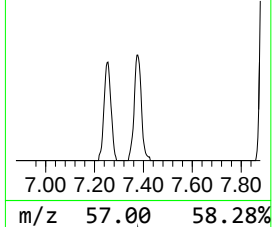
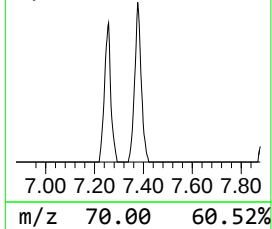
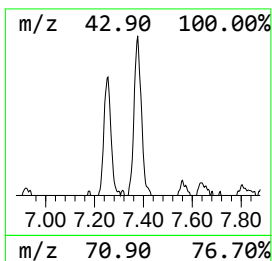
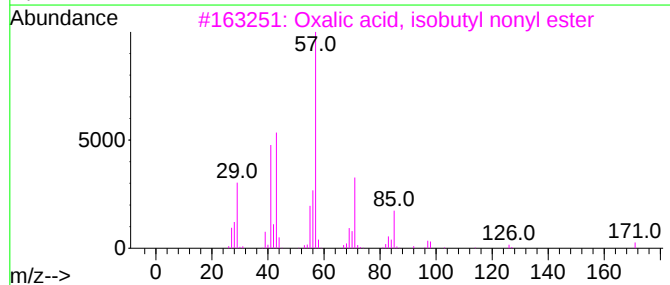
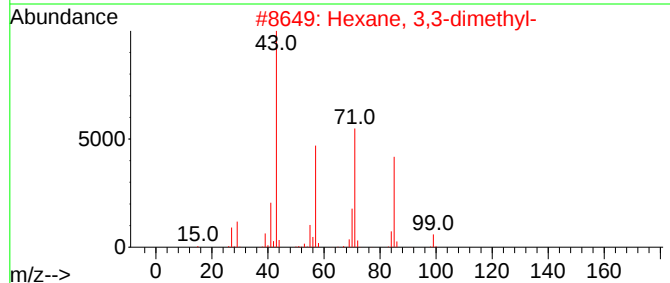
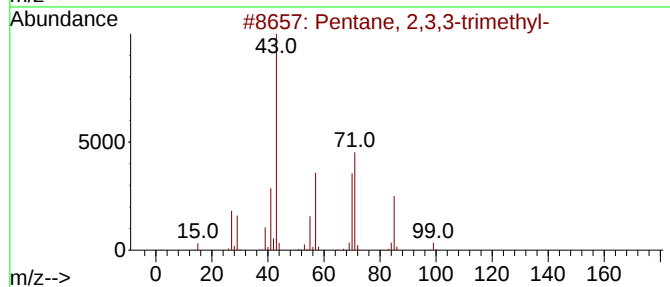
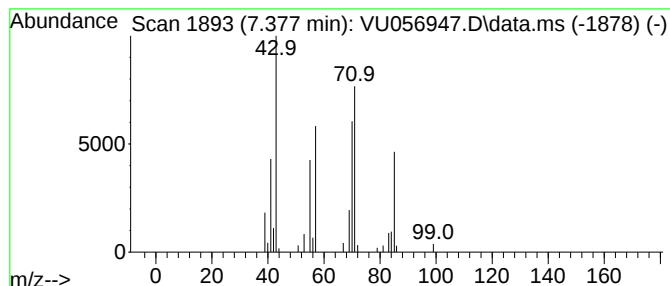
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.377	0.61 ug/L	55371	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,3,3-trimethyl-	114	C8H18	000560-21-4	72
2			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
3			Oxalic acid, isobutyl nonyl ester	272	C15H28O4	1010309-37-4	59
4			Sulfurous acid, hexyl 2-pentyl e...	236	C11H24O3S	1000309-15-6	59
5			Hexane, 2,3,4-trimethyl-	128	C9H20	000921-47-1	56



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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
(DEL) Alkane: S...	7.377	0.6	ug/L	55371	1	6.245	454880	5.0