

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090723\
 Data File : VU055218.D
 Acq On : 08 Sep 2023 04:32
 Operator : MD/SY
 Sample : 04307-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4N7

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\SFAMUTR090123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU055218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.354	14	20	25	rBV	7988	8630	1.49%	0.141%
2	1.480	52	59	66	rBV	57091	56946	9.84%	0.927%
3	1.595	86	95	107	rVB	49490	57734	9.98%	0.940%
4	1.911	184	193	204	rVB	60684	78359	13.54%	1.276%
5	2.563	384	396	408	rBV	105907	171920	29.72%	2.800%
6	2.634	408	418	445	rVB	50768	112795	19.50%	1.837%
7	2.952	507	517	534	rVV	14863	29317	5.07%	0.477%
8	3.042	535	545	556	rVB4	9870	18566	3.21%	0.302%
9	3.206	593	596	612	rVB2	4383	7343	1.27%	0.120%
10	4.441	966	980	989	rBV6	4065	10452	1.81%	0.170%
11	4.663	1024	1049	1082	rBV3	140100	540449	93.42%	8.802%
12	4.817	1092	1097	1116	rVB3	5879	14000	2.42%	0.228%
13	5.062	1157	1173	1202	rBV	131620	306676	53.01%	4.994%
14	5.724	1358	1379	1397	rBV3	218286	574577	99.32%	9.357%
15	6.248	1529	1542	1568	rBV	204513	403315	69.71%	6.568%
16	6.541	1621	1633	1653	rBV	89240	176871	30.57%	2.880%
17	6.688	1666	1679	1698	rBV2	143954	288708	49.90%	4.702%
18	7.123	1807	1814	1824	rBV5	3552	6297	1.09%	0.103%
19	7.566	1941	1952	1968	rBV2	45878	83210	14.38%	1.355%
20	7.795	2012	2023	2037	rBV4	12112	24585	4.25%	0.400%
21	7.897	2042	2055	2072	rVV	251128	454077	78.49%	7.395%
22	7.971	2072	2078	2097	rVB2	9317	18053	3.12%	0.294%
23	8.180	2131	2143	2158	rBV2	26653	48470	8.38%	0.789%
24	8.637	2273	2285	2320	rBV5	220990	578525	100.00%	9.422%
25	8.788	2324	2332	2338	rVV4	11401	18093	3.13%	0.295%
26	8.836	2338	2347	2362	rVB	64513	110381	19.08%	1.798%
27	9.415	2515	2527	2546	rBV	311098	541675	93.63%	8.822%
28	9.695	2608	2614	2625	rVB5	3632	6214	1.07%	0.101%
29	10.122	2733	2747	2761	rVB5	6160	16839	2.91%	0.274%
30	10.245	2771	2785	2797	rBV3	7165	13590	2.35%	0.221%
31	10.756	2932	2944	2957	rBV	107882	175392	30.32%	2.856%
32	11.055	3025	3037	3046	rBV5	2842	5890	1.02%	0.096%
33	11.691	3225	3235	3243	rBV6	3834	5886	1.02%	0.096%
34	11.810	3259	3272	3290	rBV	335360	557232	96.32%	9.075%
35	12.061	3338	3350	3369	rBV2	51760	112088	19.37%	1.825%
36	12.193	3379	3391	3406	rVB	248805	415468	71.82%	6.766%

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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\SFAMUTR090123WMA.M
Title : TRACE VOA SFAM1.0

37	12.775	3563	3572	3584	rVB8	6595	11577	2.00%	0.189%
38	12.891	3597	3608	3621	rVB8	11095	19021	3.29%	0.310%
39	13.843	3894	3904	3923	rVB2	29228	49344	8.53%	0.804%
40	14.331	4047	4056	4067	rVB5	7074	11794	2.04%	0.192%

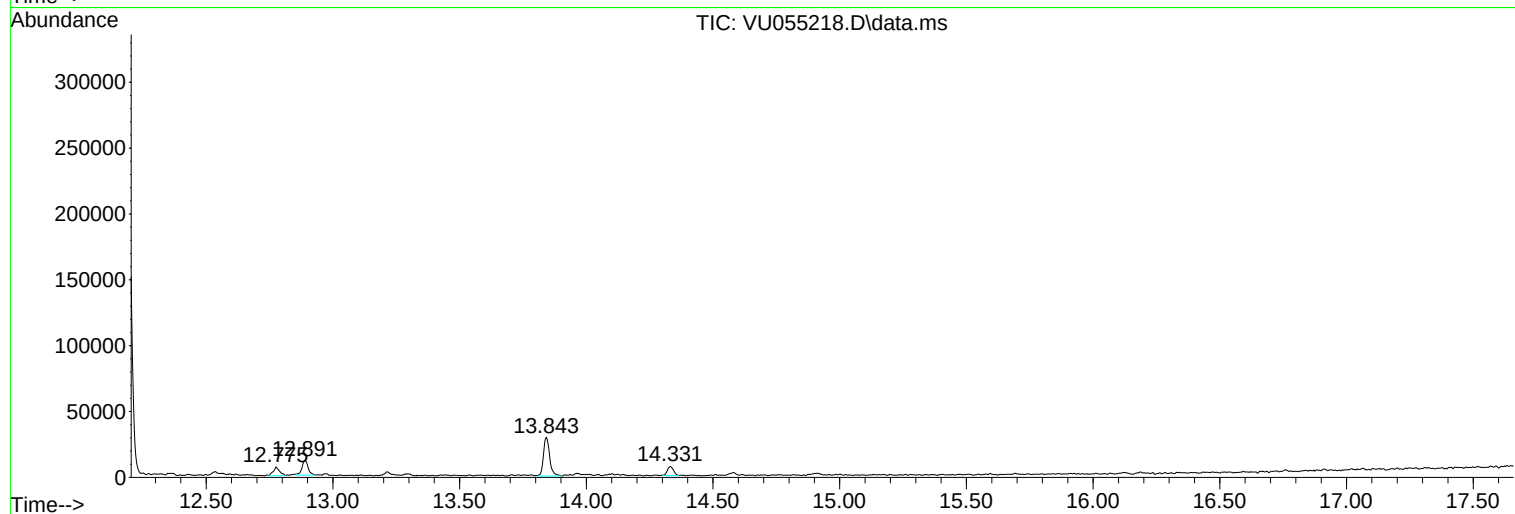
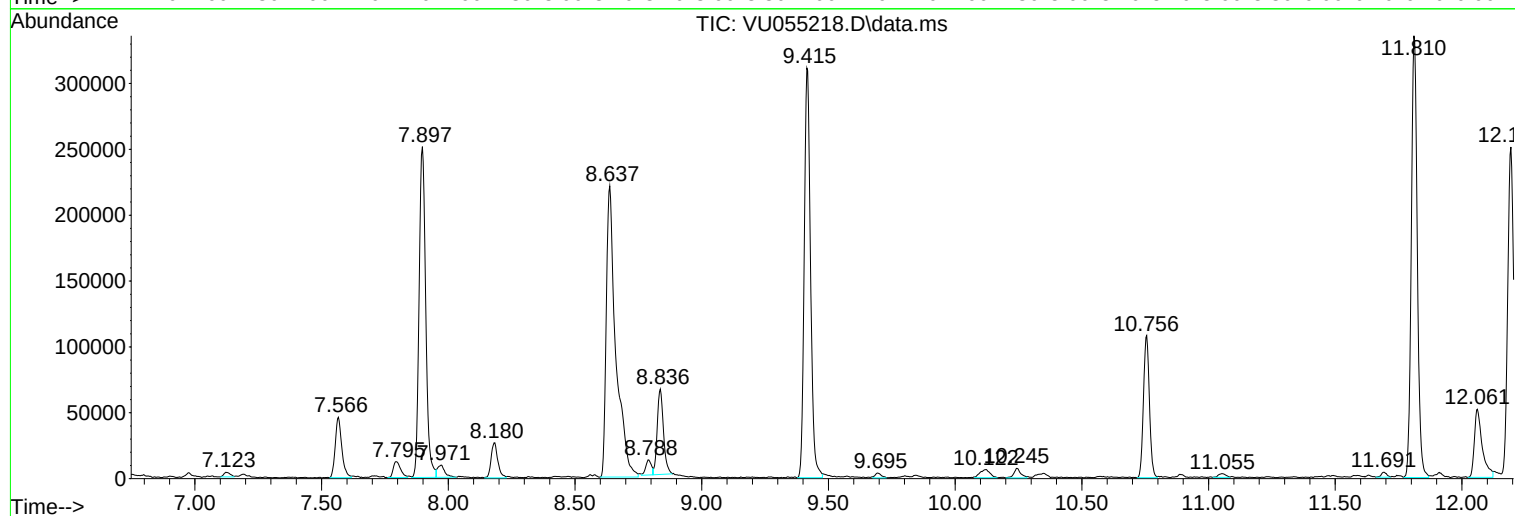
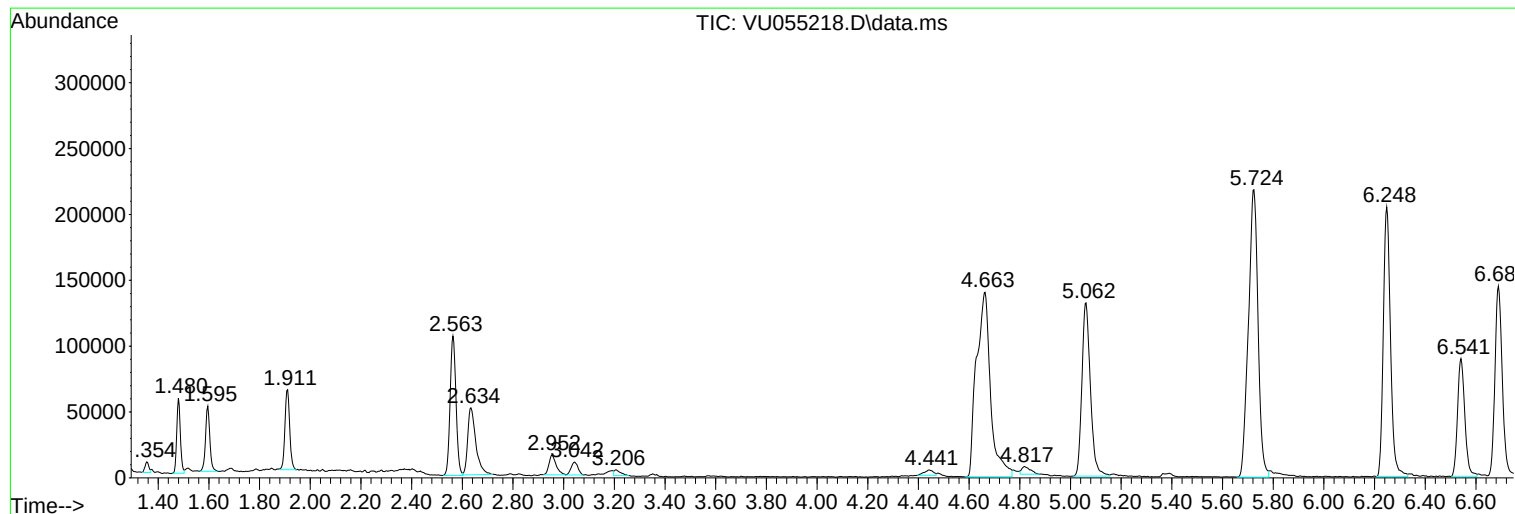
Sum of corrected areas: 6140359

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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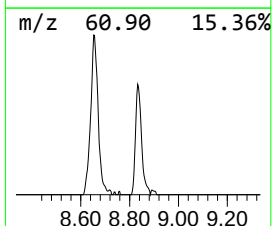
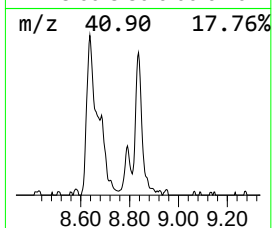
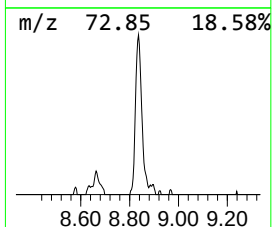
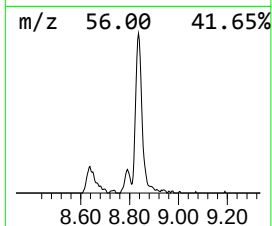
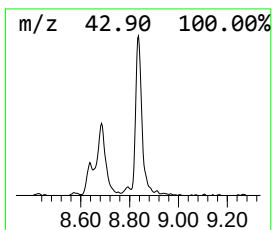
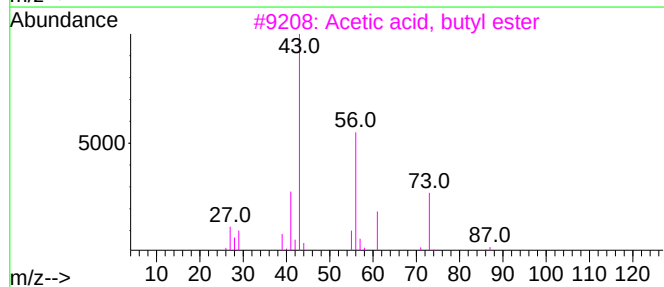
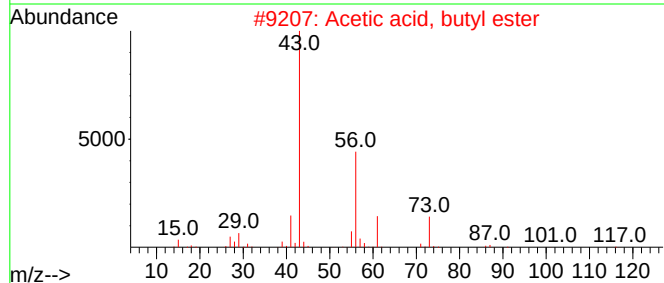
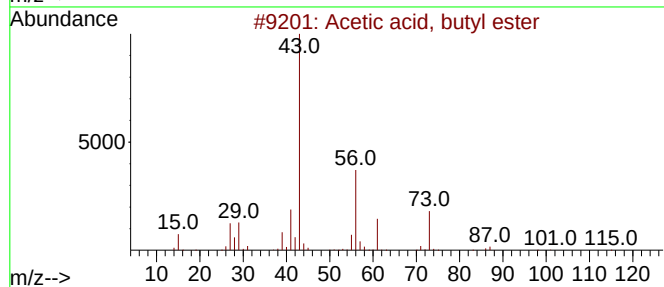
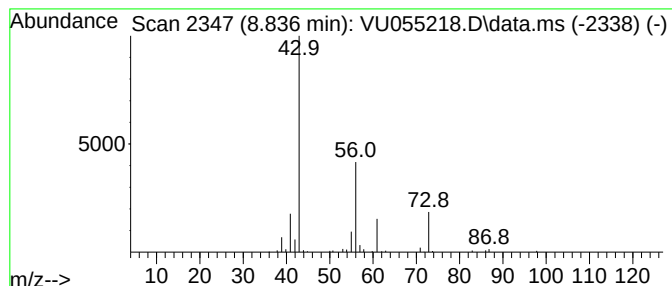
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Acetic acid, butyl ester Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.836	1.02 ug/L	110381	Chlorobenzene-d5	9.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	83	
2	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	64	
3	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	59	
4	Acetic acid, butyl ester		116	C6H12O2	000123-86-4	39	
5	Acetic acid, hexyl ester		144	C8H16O2	000142-92-7	38	



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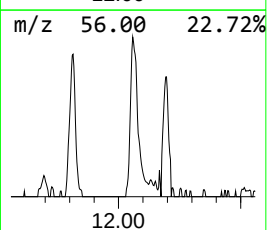
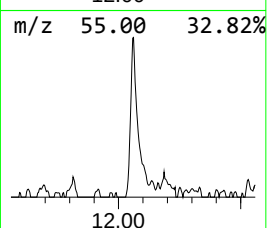
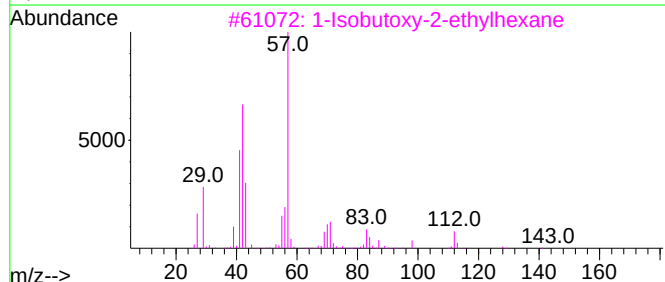
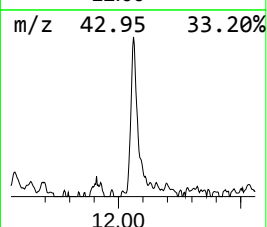
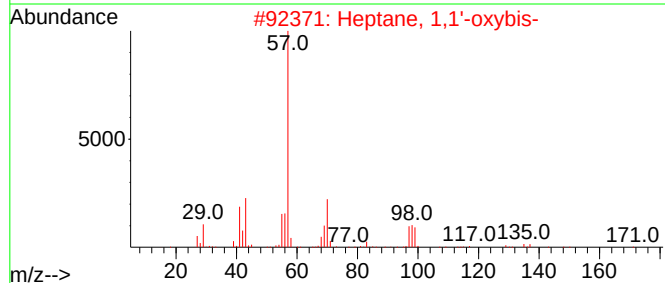
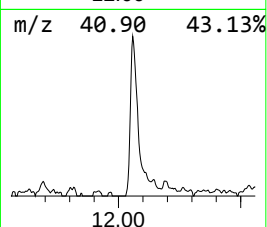
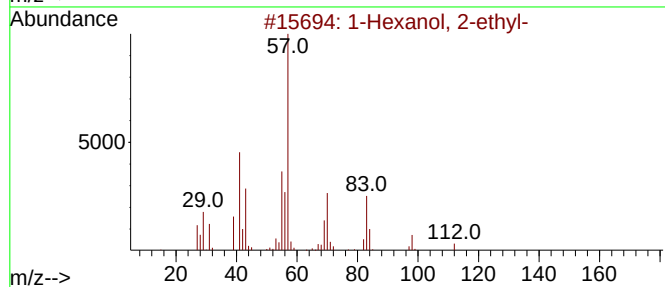
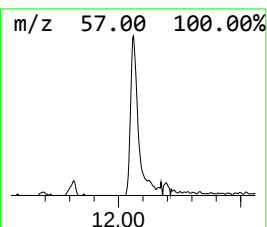
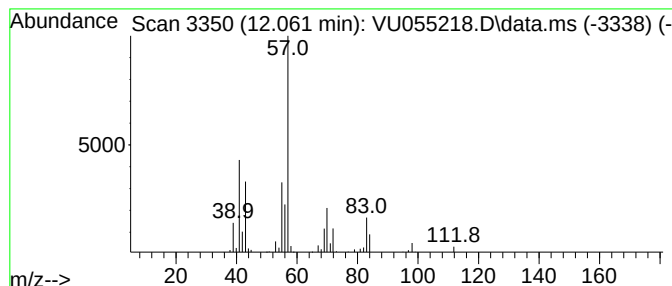
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	1.01 ug/L	112088	1,4-Dichlorobenzene-d4	11.810

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
2			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	59
3			1-Isobutoxy-2-ethylhexane	186	C12H26O	1000139-90-3	56
4			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	53
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	53



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetic acid, bu...	8.836	1.0	ug/L	110381	2	9.418	541675	5.0
1-Hexanol, 2-et...	12.061	1.0	ug/L	112088	3	11.810	557232	5.0