

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090723\
 Data File : VU055219.D
 Acq On : 08 Sep 2023 04:56
 Operator : MD/SY
 Sample : 04307-16
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH4P7

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: VU055219.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	13	20	30	rBV3	7309	9608	1.64%	0.154%
2	1.480	52	59	66	rBV	58154	59920	10.26%	0.962%
3	1.515	66	70	80	rVB2	6877	8769	1.50%	0.141%
4	1.596	85	95	109	rVB	49925	68661	11.75%	1.102%
5	1.686	116	123	133	rBV2	5504	9110	1.56%	0.146%
6	1.911	184	193	201	rBV	60738	78203	13.38%	1.255%
7	2.563	380	396	408	rBV	106321	173677	29.72%	2.788%
8	2.634	408	418	452	rVB	56889	130262	22.29%	2.091%
9	2.952	508	517	533	rVV2	15012	29491	5.05%	0.473%
10	3.042	536	545	559	rVB3	11231	19712	3.37%	0.316%
11	4.435	962	978	992	rBV6	9428	28272	4.84%	0.454%
12	4.660	1025	1048	1086	rBV3	130735	512205	87.66%	8.223%
13	5.062	1158	1173	1197	rBV2	129598	300523	51.43%	4.825%
14	5.724	1360	1379	1399	rBV2	219148	576526	98.67%	9.255%
15	6.248	1528	1542	1570	rBV	206356	407832	69.80%	6.547%
16	6.541	1621	1633	1648	rBV2	81235	157854	27.02%	2.534%
17	6.689	1665	1679	1699	rBV	141500	282042	48.27%	4.528%
18	7.126	1803	1815	1826	rBV5	3944	7994	1.37%	0.128%
19	7.190	1831	1835	1850	rVB6	3513	6194	1.06%	0.099%
20	7.566	1938	1952	1971	rBV	44903	84822	14.52%	1.362%
21	7.791	2013	2022	2041	rBV2	13648	25977	4.45%	0.417%
22	7.898	2041	2055	2070	rVV	253867	453098	77.55%	7.274%
23	7.971	2072	2078	2092	rVB3	9532	17174	2.94%	0.276%
24	8.180	2133	2143	2160	rBV2	28024	48378	8.28%	0.777%
25	8.637	2273	2285	2320	rBV5	225277	584298	100.00%	9.380%
26	8.788	2324	2332	2338	rVV3	12669	20516	3.51%	0.329%
27	8.836	2339	2347	2369	rVB	66551	115716	19.80%	1.858%
28	9.415	2515	2527	2552	rBV	313620	544956	93.27%	8.749%
29	10.119	2742	2746	2761	rVB	5519	11143	1.91%	0.179%
30	10.241	2772	2784	2797	rBV4	7846	14060	2.41%	0.226%
31	10.753	2932	2943	2965	rBV	107291	178929	30.62%	2.872%
32	11.052	3025	3036	3044	rBV4	3812	6311	1.08%	0.101%
33	11.688	3224	3234	3246	rBV7	5159	8957	1.53%	0.144%
34	11.811	3258	3272	3294	rBV	347563	569987	97.55%	9.150%
35	11.910	3294	3303	3314	rVB	4004	7120	1.22%	0.114%
36	12.061	3339	3350	3375	rBV2	74199	163565	27.99%	2.626%

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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	12.193	3379	3391	3407	rVB	246745	412539	70.60%	6.623%
38	12.778	3564	3573	3582	rBV5	8508	13690	2.34%	0.220%
39	12.891	3600	3608	3620	rVB6	13215	20598	3.53%	0.331%
40	13.212	3697	3708	3713	rBV8	3766	6657	1.14%	0.107%
41	13.843	3893	3904	3918	rBV	26561	43356	7.42%	0.696%
42	14.331	4045	4056	4065	rVB6	6356	10387	1.78%	0.167%

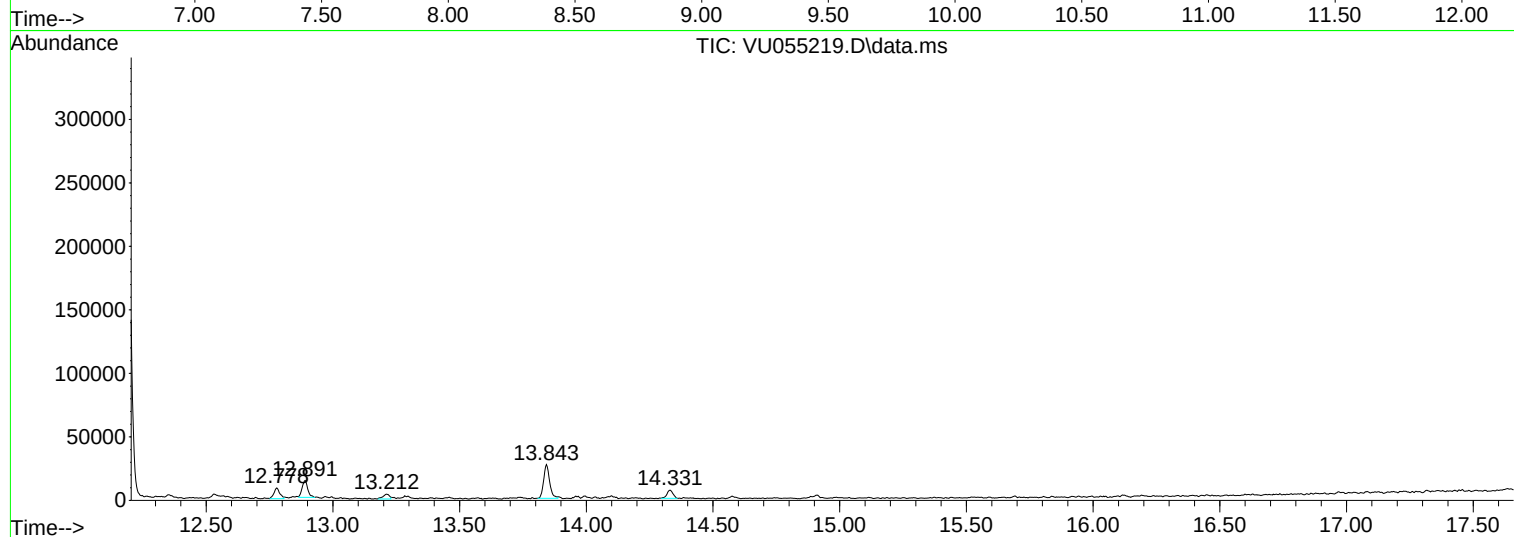
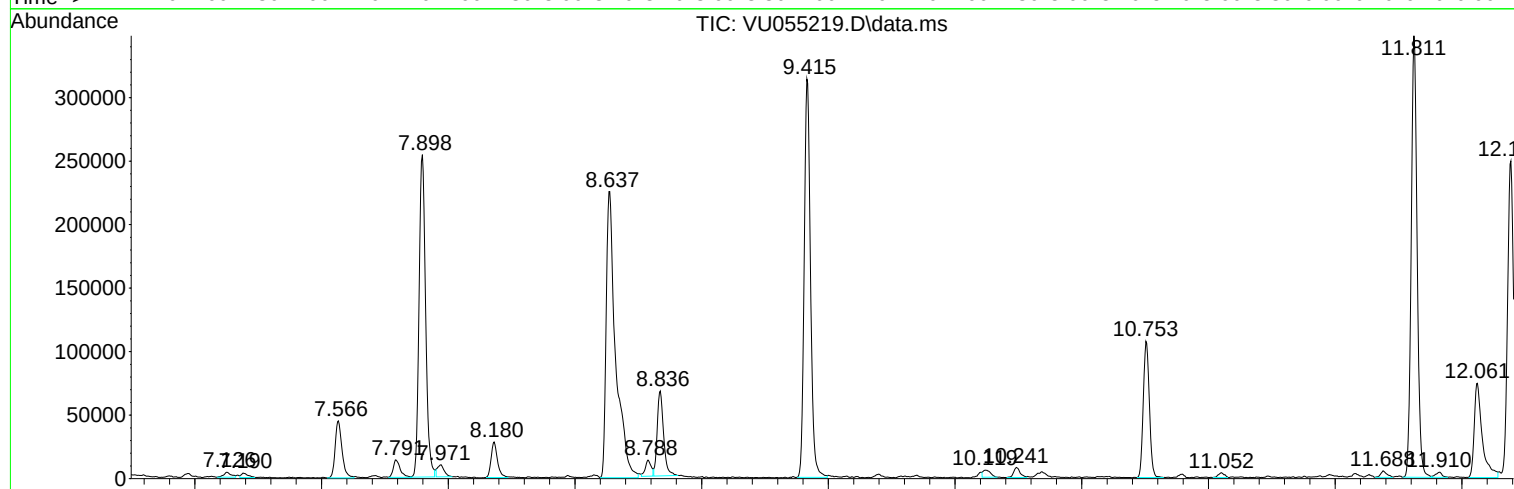
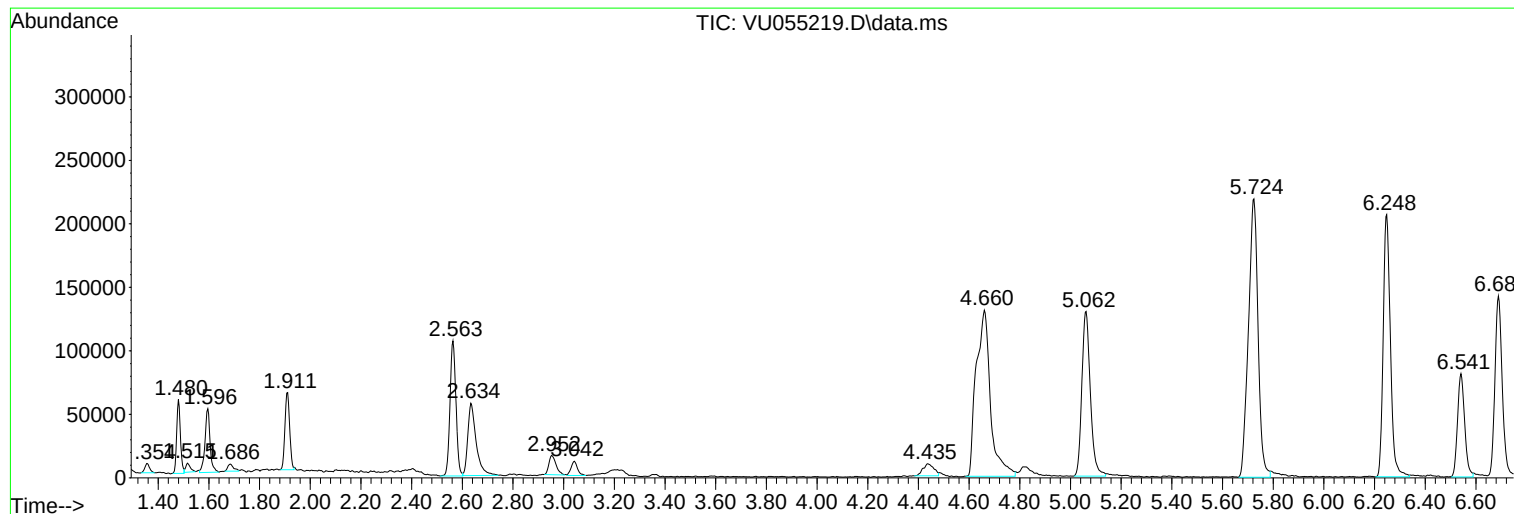
Sum of corrected areas: 6229089

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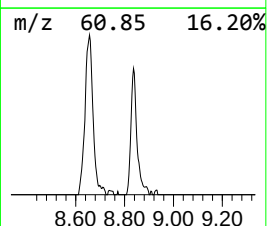
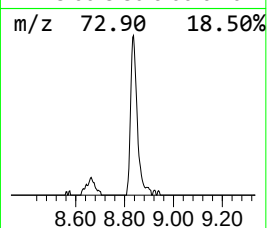
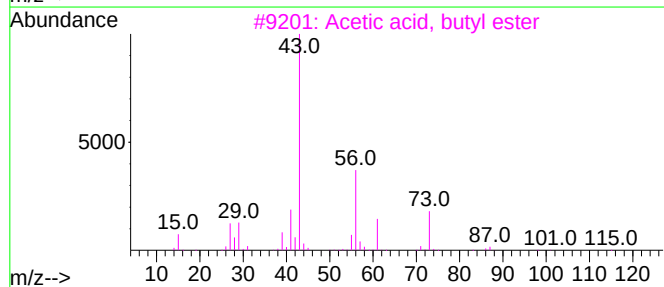
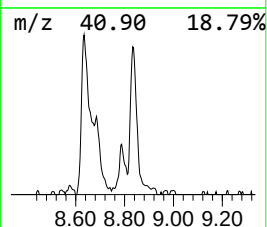
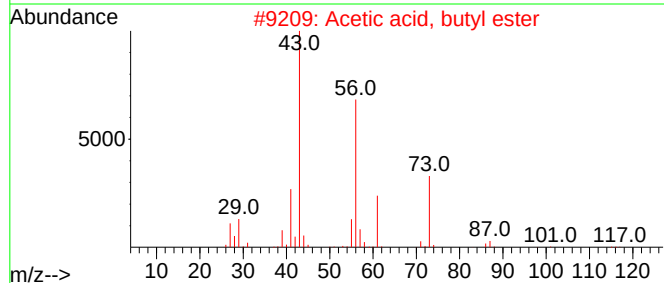
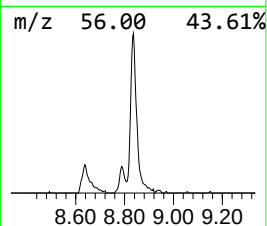
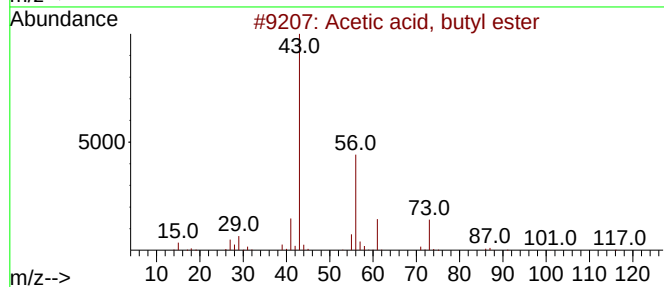
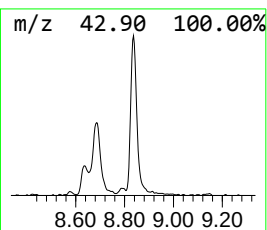
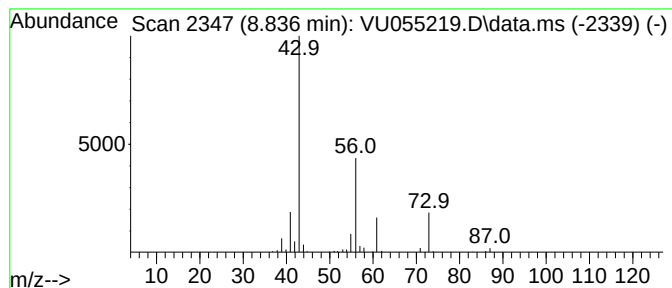
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR090123WMA.M
Quant Title : TRACE VOA SFAM1.0

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	1.06 ug/L	115716	Chlorobenzene-d5	9.418

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
2			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	78
3			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	74
4			Acetic acid, butyl ester	116	C6H12O2	000123-86-4	64
5			Isobutyl acetate	116	C6H12O2	000110-19-0	39



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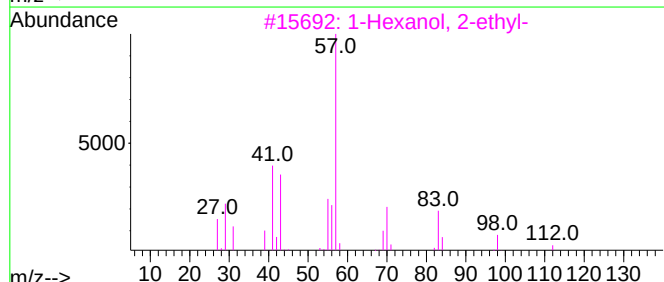
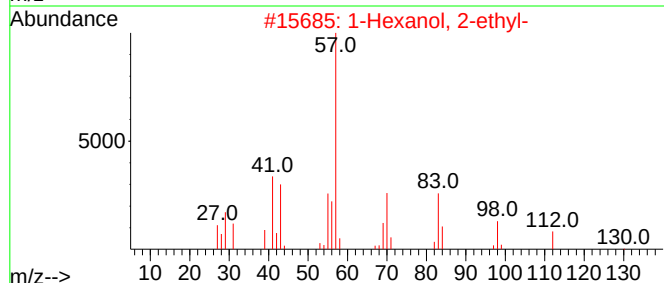
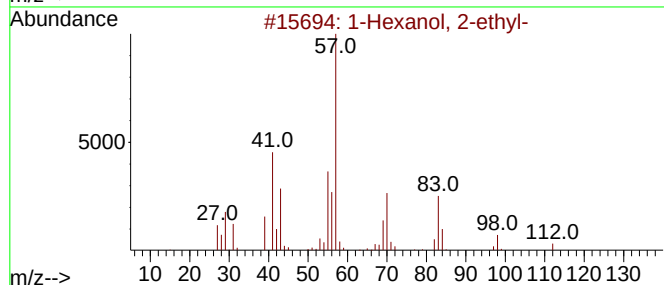
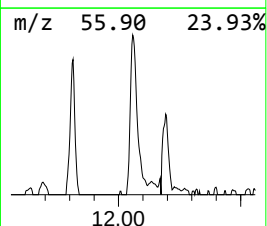
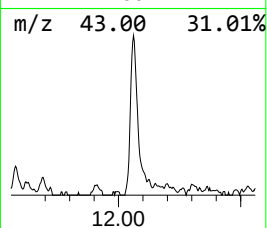
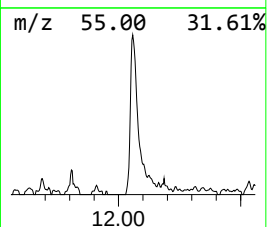
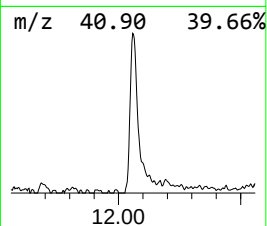
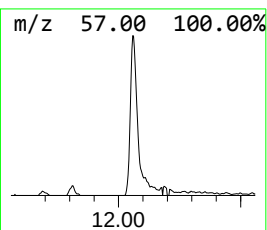
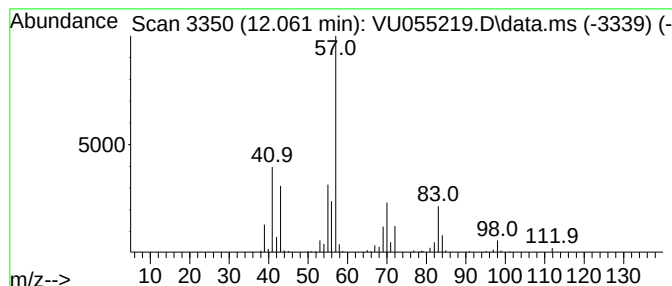
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	1.43 ug/L	163565	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	86
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	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	1.1	ug/L	115716	2	9.418	544956	5.0
1-Hexanol, 2-et...	12.061	1.4	ug/L	163565	3	11.810	569987	5.0