

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112322\
 Data File : VU052105.D
 Acq On : 23 Nov 2022 22:51
 Operator : JC/MD
 Sample : N5739-03
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBNK3

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\SFAMUTR111822WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU052105.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.491	30	47	53	rBV4	13051	29504	3.31%	0.407%
2	1.520	53	56	67	rVV4	5756	10871	1.22%	0.150%
3	1.584	69	76	94	rVB2	288904	418402	46.90%	5.776%
4	1.684	101	107	119	rVB	9911	13209	1.48%	0.182%
5	1.768	125	133	141	rBV4	8850	13043	1.46%	0.180%
6	1.912	169	178	192	rBV	88144	123372	13.83%	1.703%
7	2.568	369	382	393	rBV	162221	264559	29.66%	3.652%
8	2.623	393	399	413	rVB	10240	18225	2.04%	0.252%
9	3.166	554	568	592	rBV2	44603	103646	11.62%	1.431%
10	3.861	763	784	787	rBV	8096	21694	2.43%	0.299%
11	4.440	949	964	984	rVB5	12750	35599	3.99%	0.491%
12	4.616	1007	1019	1046	rBV	140906	346014	38.79%	4.777%
13	5.060	1140	1157	1184	rBV	162853	370093	41.49%	5.109%
14	5.722	1343	1363	1395	rBV2	306708	820241	91.95%	11.323%
15	6.247	1511	1526	1554	rBV	253303	500886	56.15%	6.915%
16	6.687	1649	1663	1684	rBV	197851	395920	44.38%	5.466%
17	7.160	1790	1810	1825	rBV2	44256	90904	10.19%	1.255%
18	7.565	1924	1936	1952	rBV	86668	156136	17.50%	2.155%
19	7.896	2026	2039	2058	rBV	335513	591199	66.27%	8.161%
20	8.179	2115	2127	2144	rBV2	54348	94833	10.63%	1.309%
21	8.629	2254	2267	2309	rBV	457129	892042	100.00%	12.314%
22	9.414	2498	2511	2538	rBV	381779	656031	73.54%	9.056%
23	10.754	2910	2928	2948	rBV	169780	275900	30.93%	3.809%
24	11.809	3244	3256	3276	rBV	304121	494049	55.38%	6.820%
25	12.192	3361	3375	3397	rBV	306518	507534	56.90%	7.006%

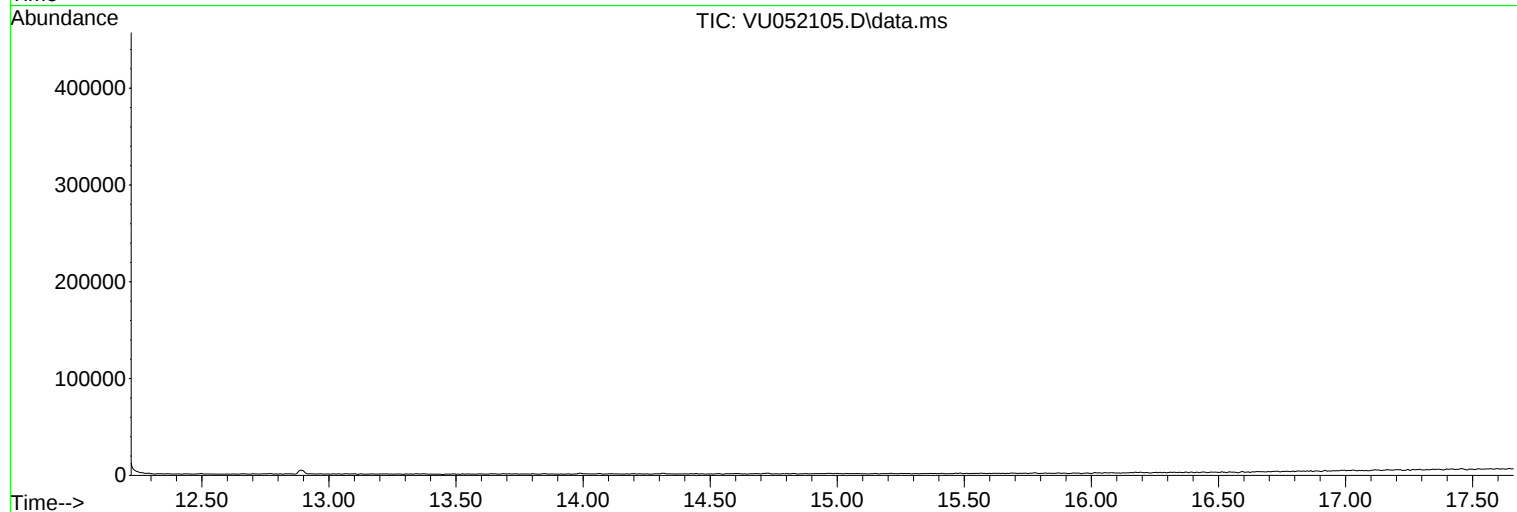
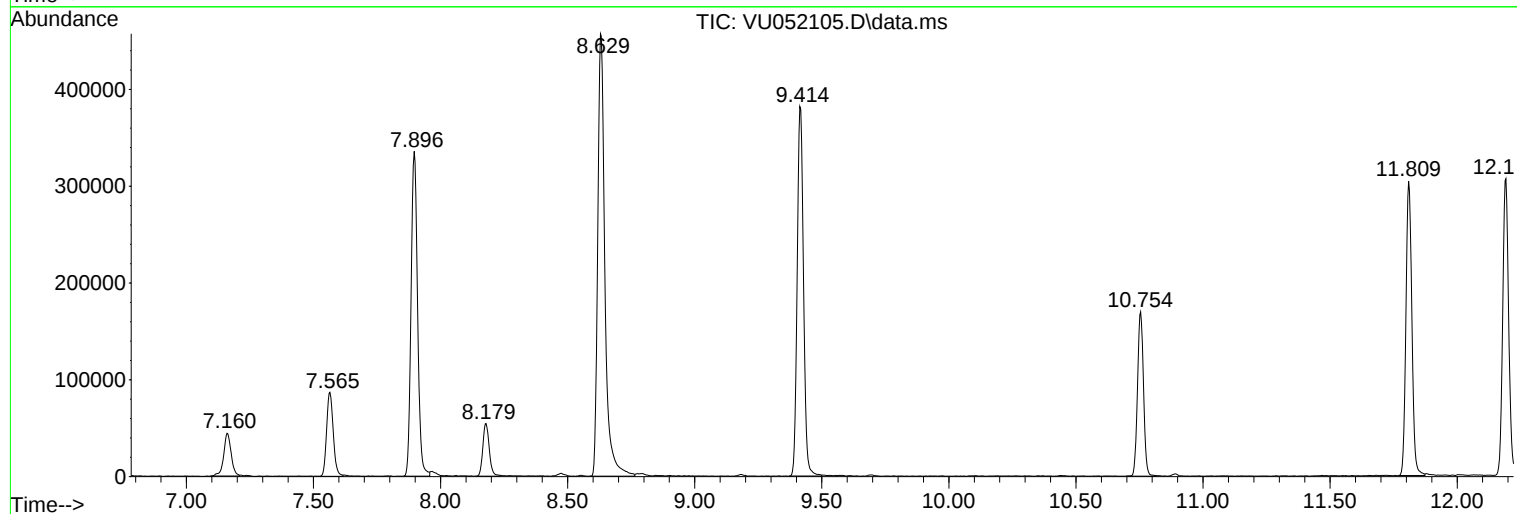
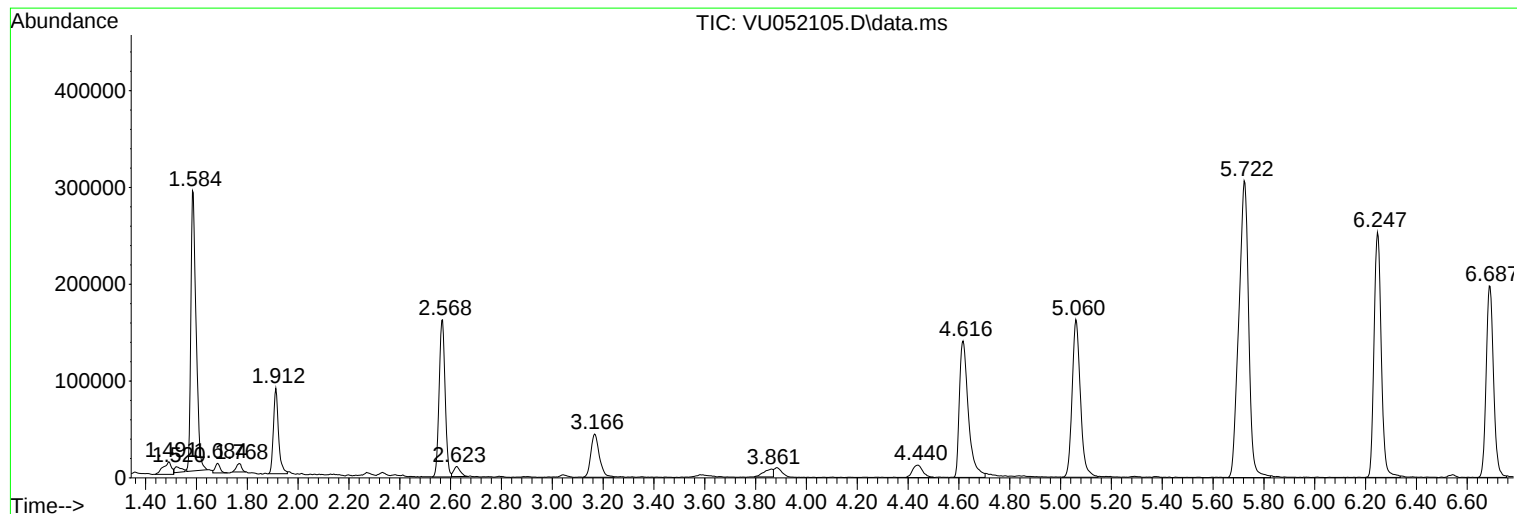
Sum of corrected areas: 7243906

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ClientSampleId :
GBNK3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.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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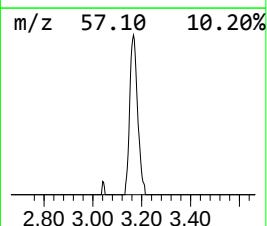
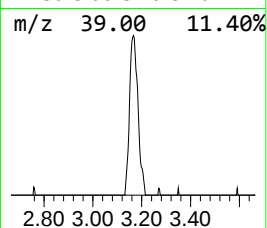
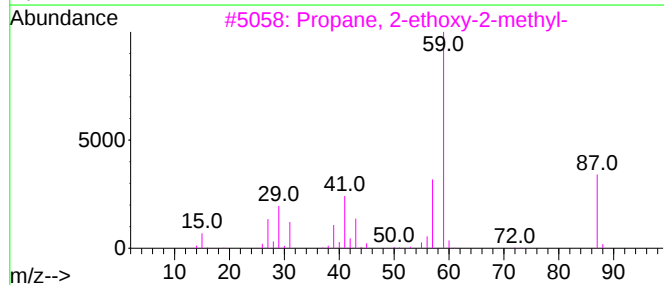
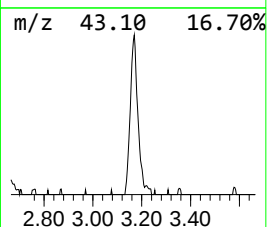
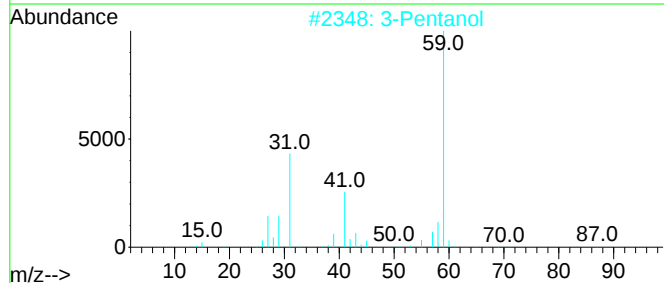
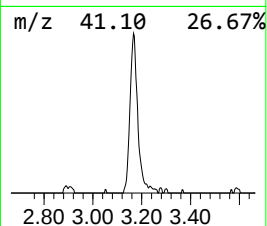
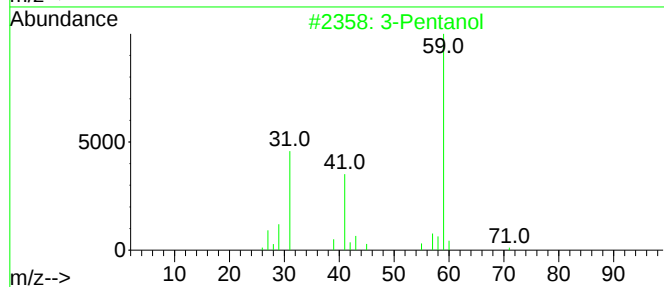
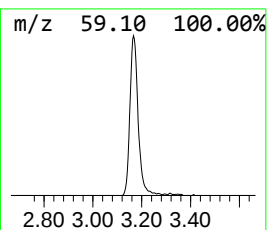
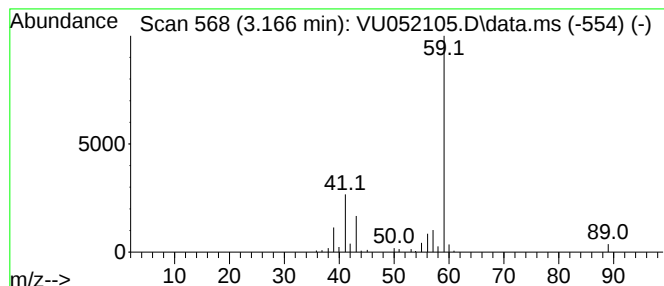
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 3-Pentanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.166	1.03 ug/L	103646	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol	88	C5H12O	000584-02-1	56
2			3-Pentanol	88	C5H12O	000584-02-1	40
3			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39
4			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanediol, 2,3-dimethyl-	118	C6H14O2	000076-09-5	9



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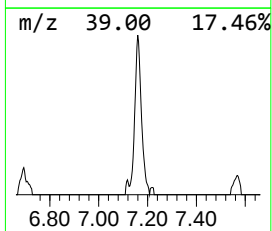
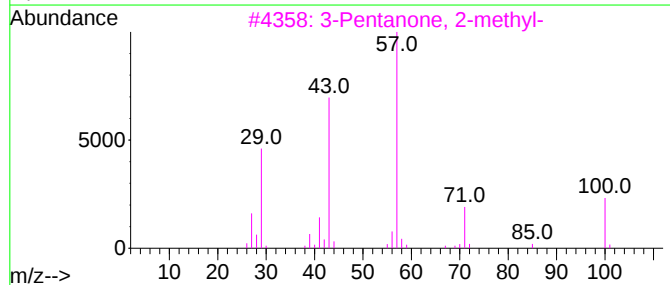
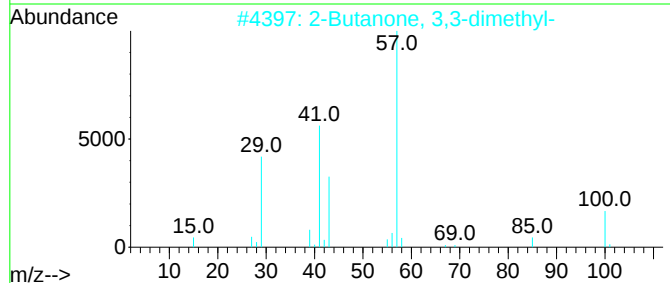
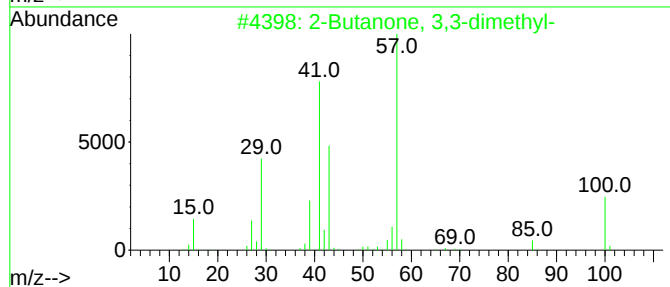
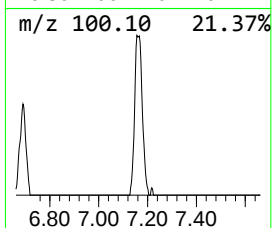
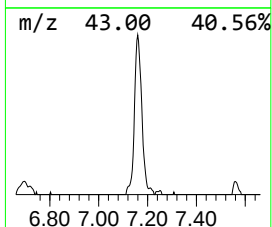
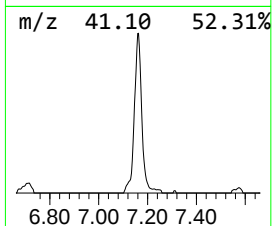
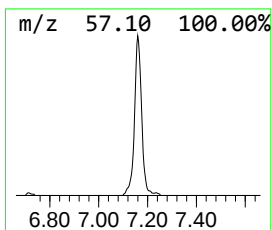
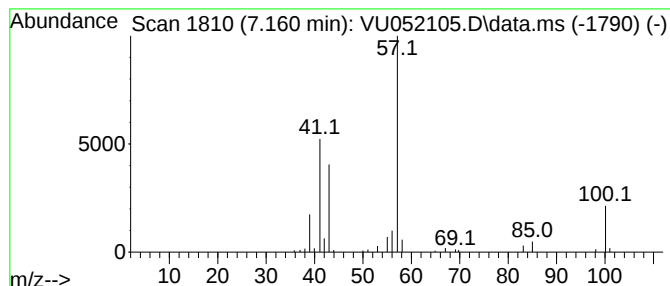
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TIC Integration Parameters: LSCINT.P

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.160	0.91 ug/L	90904	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	91
2		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	90
3		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	80
4		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	72
5		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	59



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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
3-Pentanol	3.166	1.0	ug/L	103646	1	6.247	500886	5.0
2-Butanone, 3,3...	7.160	0.9	ug/L	90904	1	6.247	500886	5.0