

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112222\
 Data File : VU052068.D
 Acq On : 23 Nov 2022 04:24
 Operator : JC/MD
 Sample : N5693-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GBN85

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: VU052068.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	69	80	93	rBV2	137478	201497	20.70%	2.525%
2	1.697	103	111	127	rVB2	7998	14264	1.47%	0.179%
3	1.916	170	179	198	rVB	102517	144361	14.83%	1.809%
4	2.565	369	381	394	rBV	197872	324500	33.33%	4.067%
5	2.658	395	410	462	rVB	81436	350122	35.96%	4.388%
6	3.047	520	531	544	rBV2	9953	18847	1.94%	0.236%
7	3.594	683	701	727	rVB3	3522	13430	1.38%	0.168%
8	3.851	757	781	782	rBV3	11000	24224	2.49%	0.304%
9	4.440	945	964	983	rBV2	54816	148498	15.25%	1.861%
10	4.642	1011	1027	1084	rBV	107361	427363	43.90%	5.356%
11	5.060	1141	1157	1187	rBV	180582	411985	42.32%	5.163%
12	5.726	1343	1364	1394	rBV2	356173	932154	95.75%	11.681%
13	6.247	1513	1526	1553	rBV	257623	498976	51.25%	6.253%
14	6.690	1648	1664	1687	rBV	221155	445524	45.76%	5.583%
15	7.128	1786	1800	1803	rBV3	12189	19539	2.01%	0.245%
16	7.166	1804	1812	1832	rVB2	30123	63185	6.49%	0.792%
17	7.565	1923	1936	1956	rBV2	96844	175628	18.04%	2.201%
18	7.896	2022	2039	2058	rBV	393288	692566	71.14%	8.679%
19	8.179	2116	2127	2146	rBV2	61014	106691	10.96%	1.337%
20	8.478	2209	2220	2235	rBV7	4546	9996	1.03%	0.125%
21	8.636	2256	2269	2300	rBV2	475266	973553	100.00%	12.200%
22	9.417	2499	2512	2545	rBV	380010	646358	66.39%	8.100%
23	9.693	2589	2598	2611	rBV3	8311	13582	1.40%	0.170%
24	10.754	2913	2928	2942	rBV	183503	299230	30.74%	3.750%
25	11.809	3244	3256	3279	rBV	289199	472518	48.54%	5.921%
26	12.192	3362	3375	3396	rBV	331545	551158	56.61%	6.907%

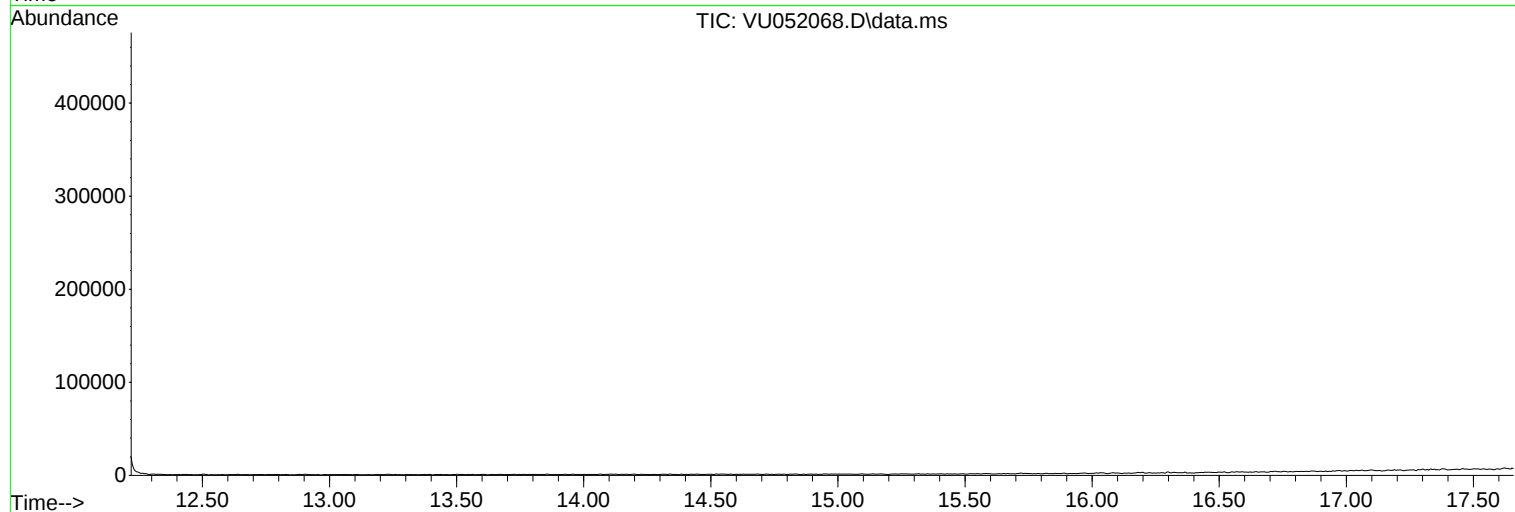
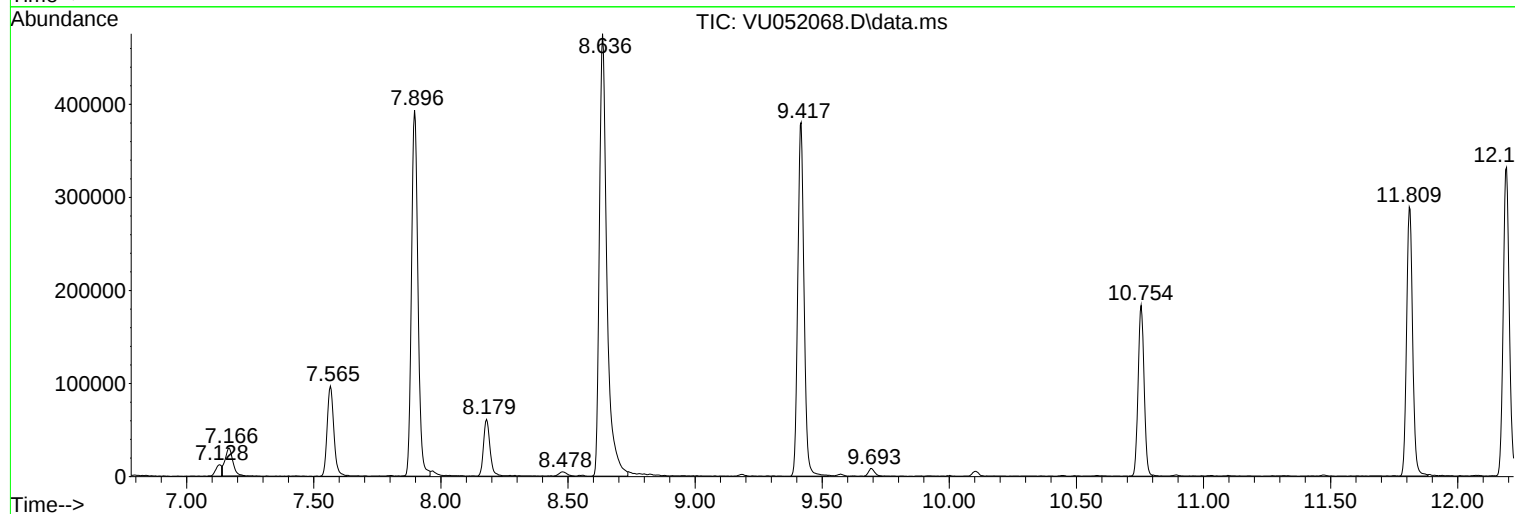
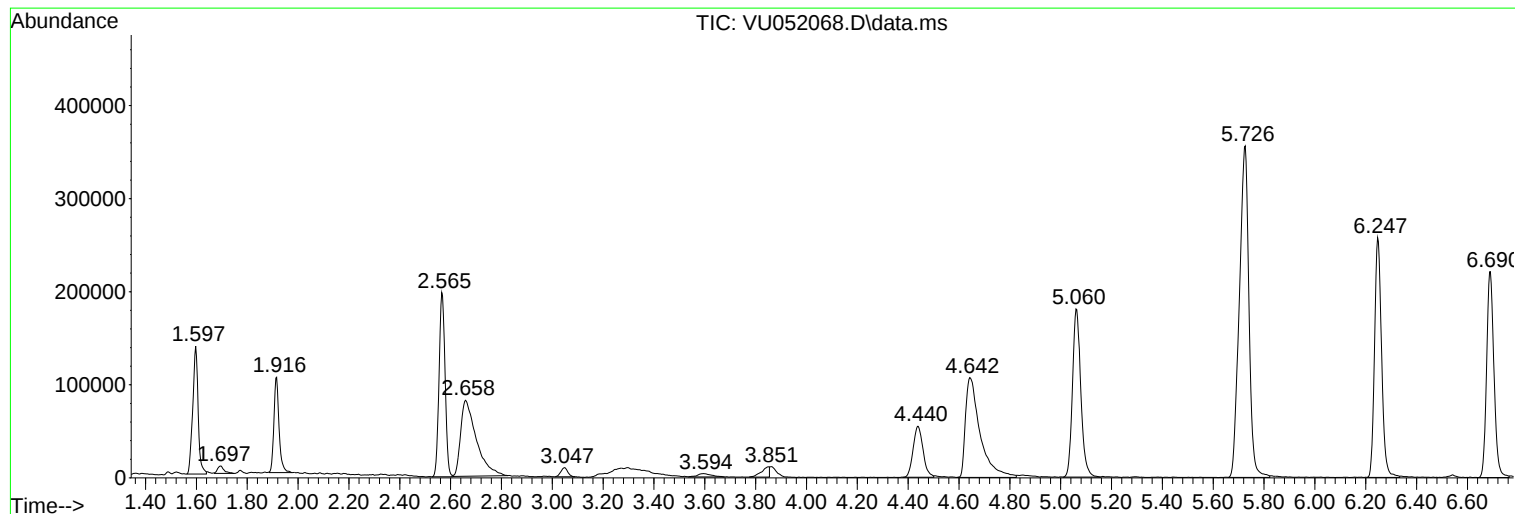
Sum of corrected areas: 7979749

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Instrument :
MSVOA_U
ClientSampleId :
GBN85

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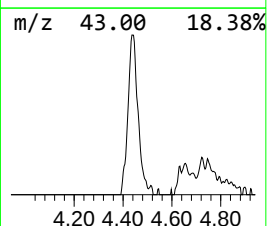
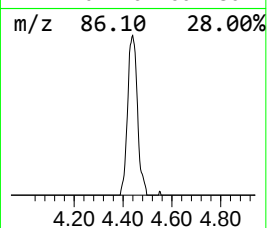
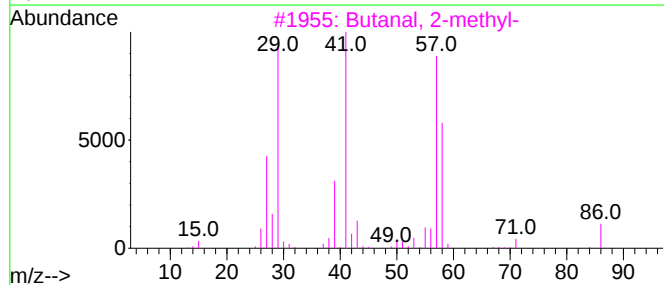
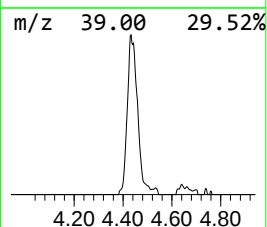
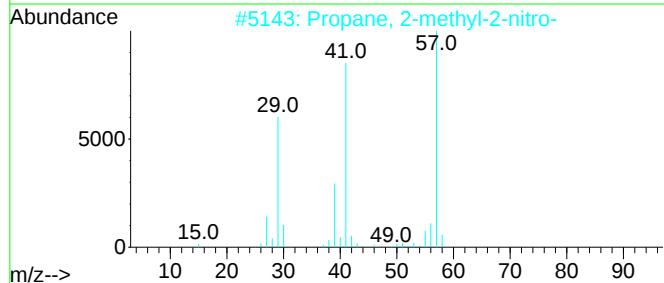
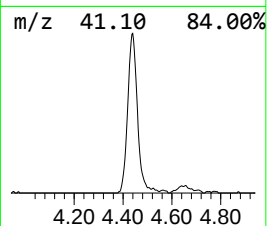
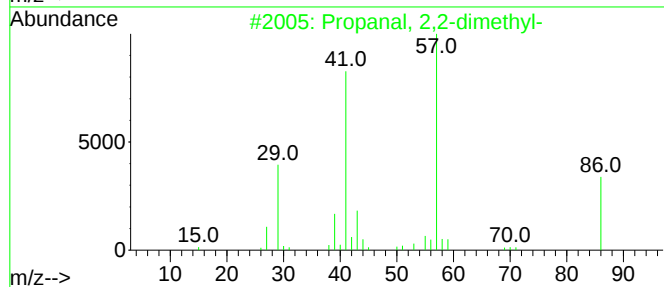
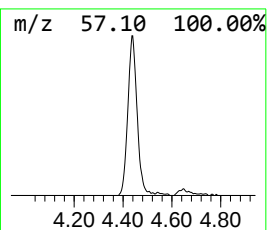
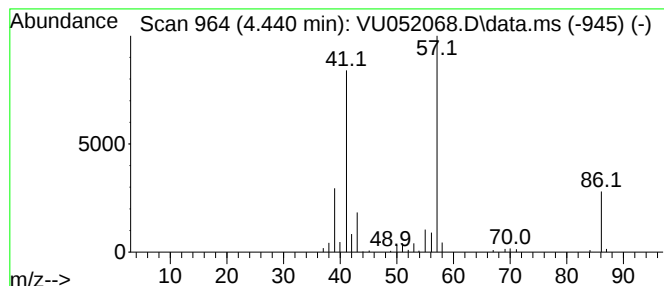
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.440	1.49 ug/L	148498	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	64
2			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
3			Butanal, 2-methyl-	86	C5H10O	000096-17-3	42
4			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	40
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40



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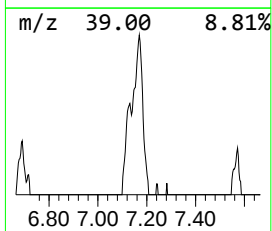
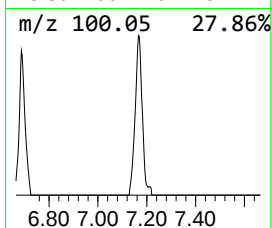
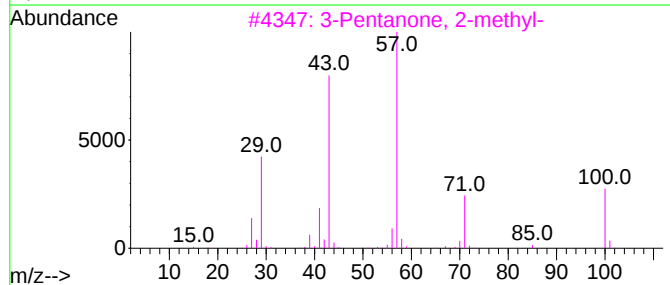
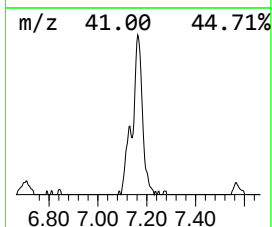
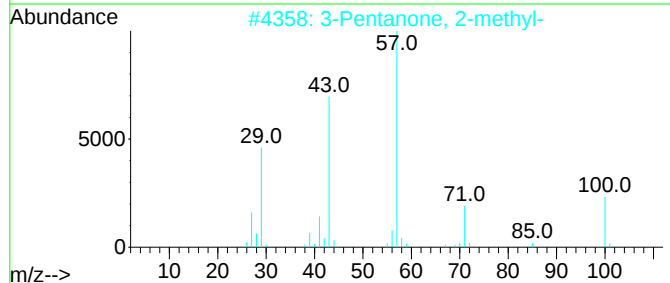
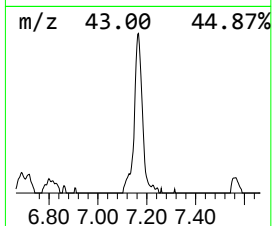
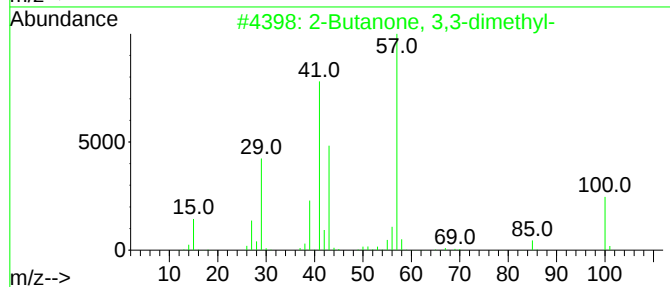
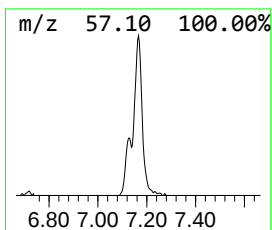
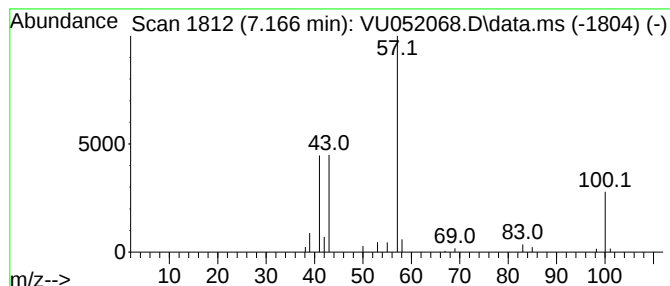
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST20.L
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.
7.166	0.63 ug/L	63185	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	64
2		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	64
3		3-Pentanone, 2-methyl-	100	C6H12O	000565-69-5	45
4		2-Butanone, 3,3-dimethyl-	100	C6H12O	000075-97-8	45
5		cis-1-Ethoxy-1-butene	100	C6H12O	1000139-43-8	33



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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
Propanal, 2,2-d...	4.440	1.5	ug/L	148498	1	6.247	498976	5.0
2-Butanone, 3,3...	7.166	0.6	ug/L	63185	1	6.247	498976	5.0