

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU111922\
 Data File : VU051947.D
 Acq On : 19 Nov 2022 11:39
 Operator : JC/MD
 Sample : N5693-04
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 50 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: VU051947.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	68	80	96	rBV2	137852	198662	22.07%	2.418%
2	1.687	100	108	116	rBV	14699	19706	2.19%	0.240%
3	1.909	169	177	201	rVB	103267	150317	16.70%	1.830%
4	2.565	368	381	391	rBV	198199	320483	35.60%	3.901%
5	2.626	391	400	430	rVB	300045	547006	60.76%	6.659%
6	3.044	517	530	549	rBV	96363	188765	20.97%	2.298%
7	3.189	559	575	602	rBV2	38379	109983	12.22%	1.339%
8	3.848	755	780	782	rBV3	10600	22733	2.53%	0.277%
9	4.436	942	963	983	rBV3	55896	149071	16.56%	1.815%
10	4.623	1008	1021	1049	rBV	136674	350820	38.97%	4.271%
11	5.060	1139	1157	1192	rBV	169307	388150	43.12%	4.725%
12	5.723	1343	1363	1393	rBV2	343604	900248	100.00%	10.959%
13	6.247	1513	1526	1557	rBV2	272611	522801	58.07%	6.364%
14	6.543	1603	1618	1634	rBV2	20297	37787	4.20%	0.460%
15	6.687	1647	1663	1691	rBV2	212182	421639	46.84%	5.133%
16	7.124	1786	1799	1803	rBV2	12803	21314	2.37%	0.259%
17	7.163	1804	1811	1831	rVB2	30723	59663	6.63%	0.726%
18	7.565	1922	1936	1952	rBV2	93325	167126	18.56%	2.035%
19	7.896	2023	2039	2058	rBV	381250	672869	74.74%	8.191%
20	8.179	2114	2127	2147	rBV	56132	98119	10.90%	1.194%
21	8.472	2209	2218	2233	rVB8	5037	10899	1.21%	0.133%
22	8.632	2256	2268	2300	rBV2	445115	869716	96.61%	10.587%
23	9.414	2498	2511	2537	rBV	392820	668278	74.23%	8.135%
24	9.693	2590	2598	2608	rBV3	8055	12163	1.35%	0.148%
25	10.755	2916	2928	2944	rBV	172364	277319	30.80%	3.376%
26	11.809	3245	3256	3278	rBV	305451	499658	55.50%	6.083%
27	12.192	3358	3375	3390	rBV	326277	529301	58.80%	6.443%

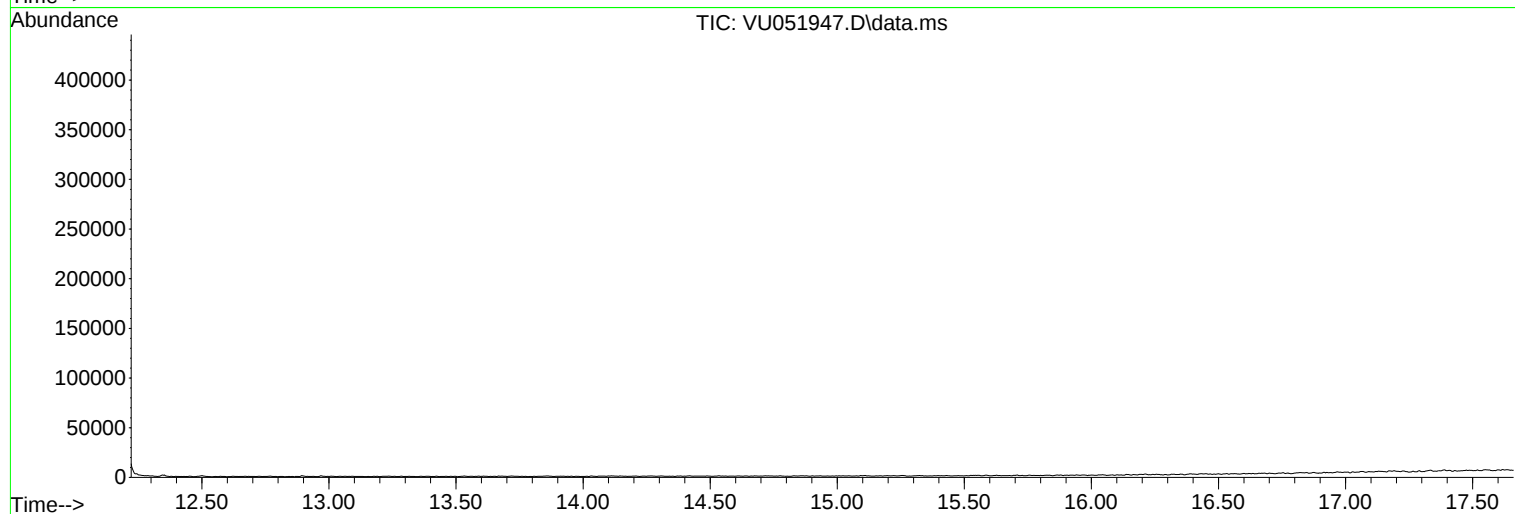
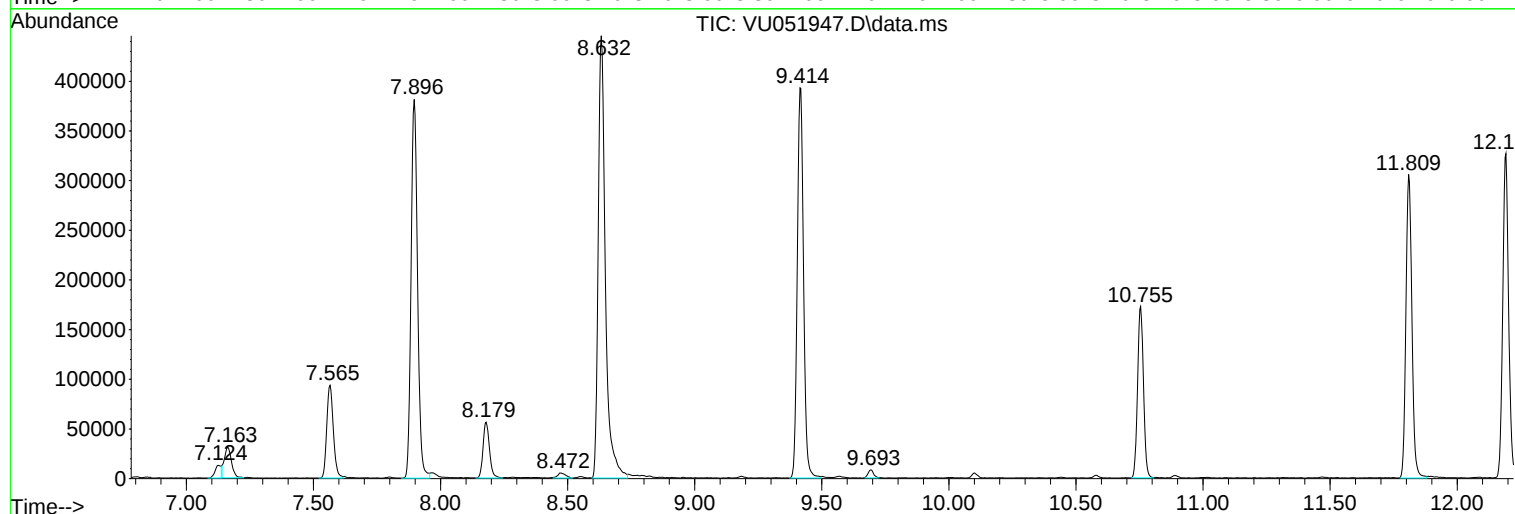
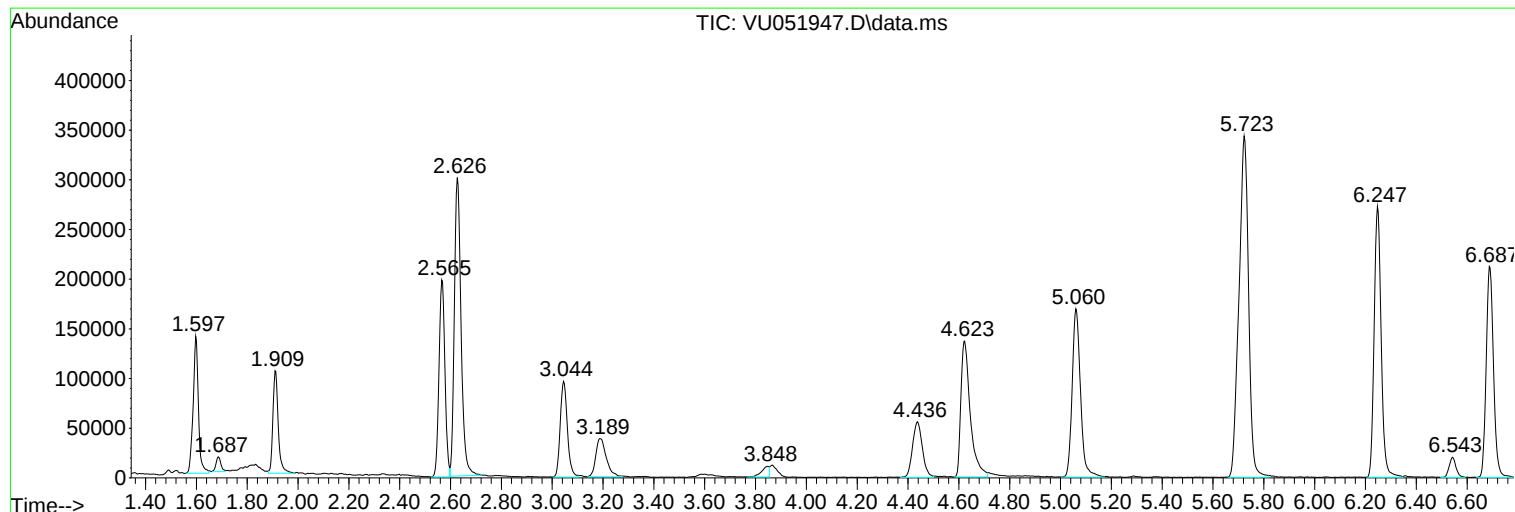
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Instrument :
MSVOA_U
ClientSampleId :
GBN85

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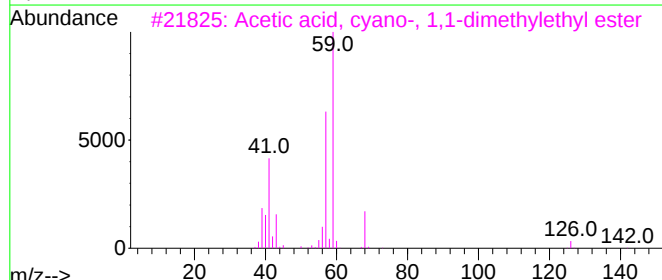
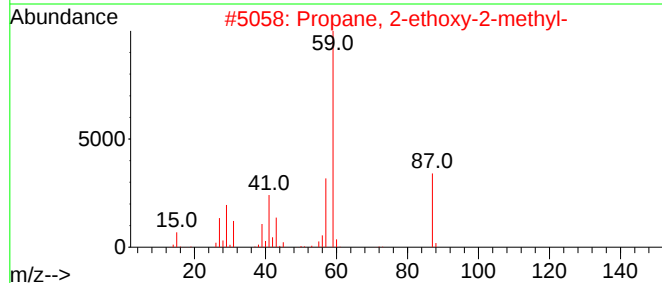
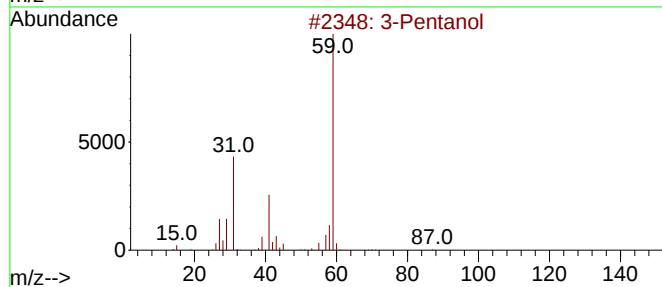
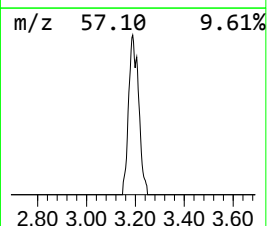
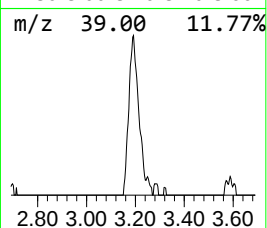
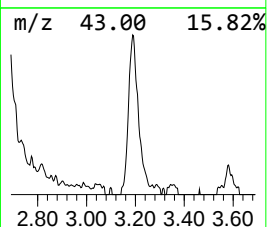
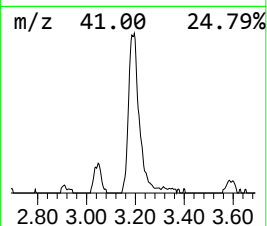
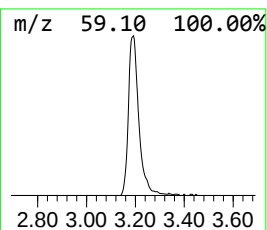
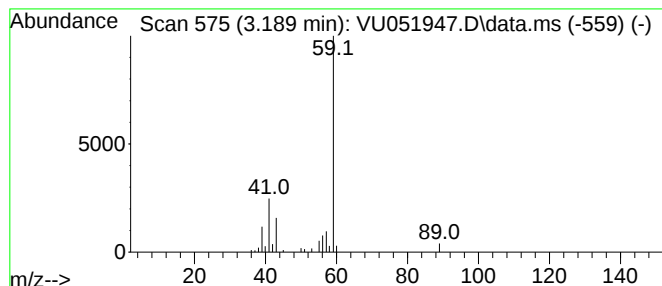
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.189	1.05 ug/L	109983	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Pentanol	88	C5H12O	000584-02-1	40
2			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
4			Pentanamide	101	C5H11NO	000626-97-1	9
5			1-Butanol, 3-methoxy-	104	C5H12O2	002517-43-3	9



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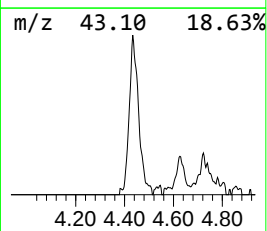
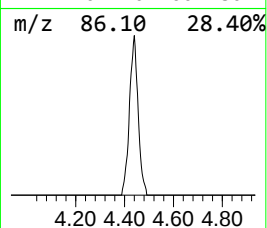
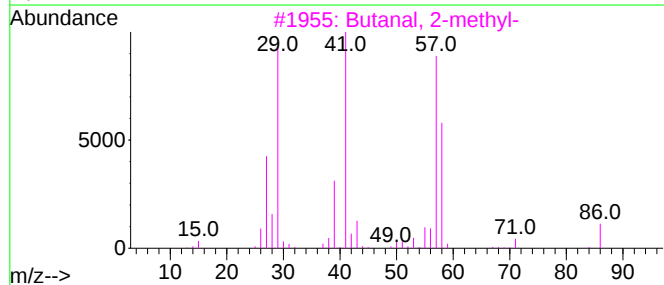
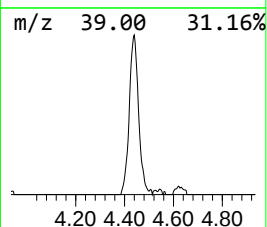
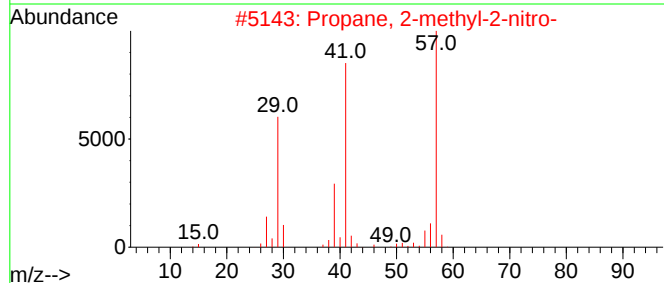
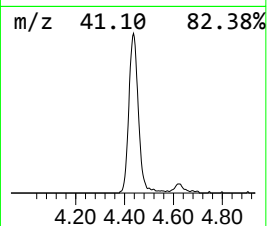
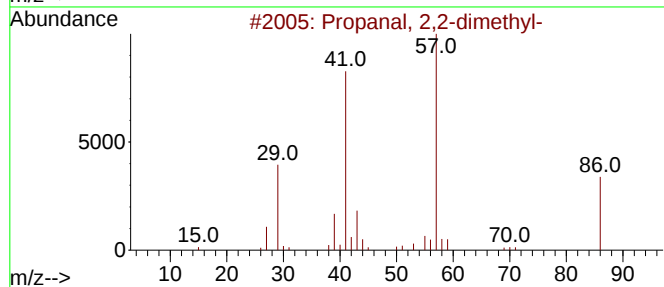
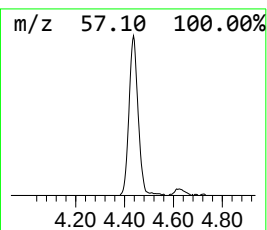
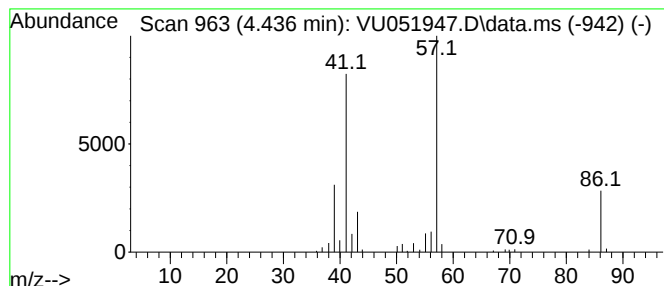
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.436	1.43 ug/L	149071	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	40
4			3-Pentanone	86	C5H10O	000096-22-0	37
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	37



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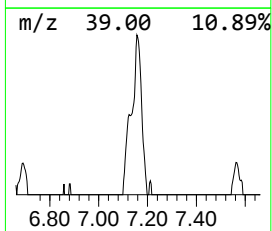
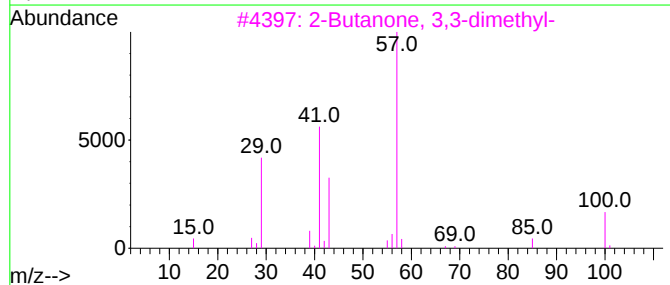
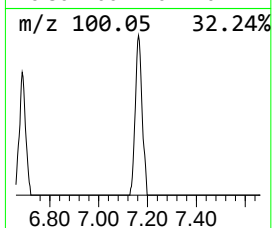
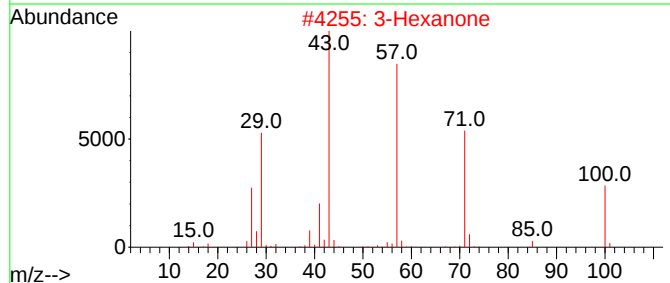
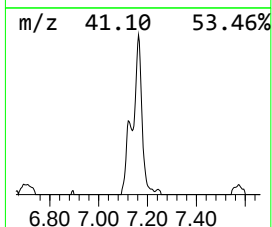
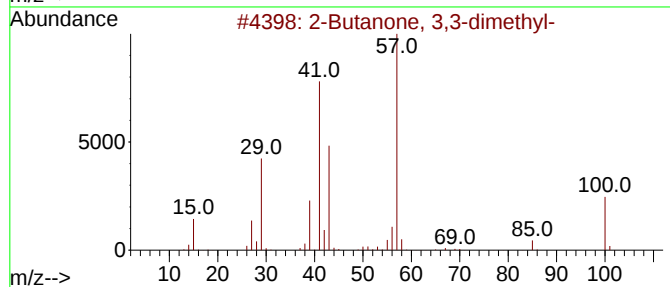
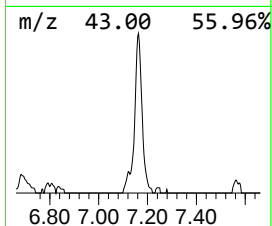
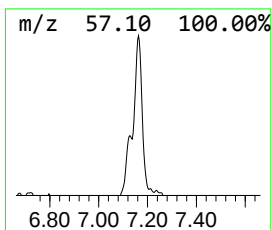
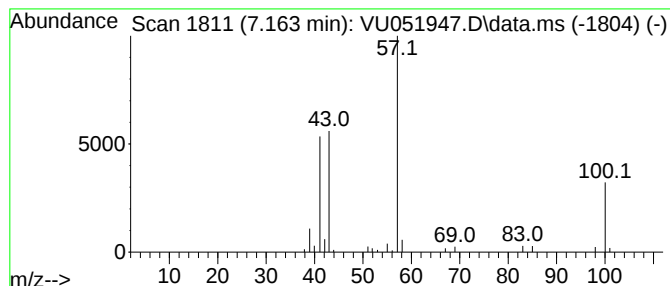
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR111822WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 2-Butanone, 3,3-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.163	0.57 ug/L	59663	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	72
2	3-Hexanone			100	C6H12O	000589-38-8	59
3	2-Butanone, 3,3-dimethyl-			100	C6H12O	000075-97-8	56
4	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	50
5	3-Pentanone, 2-methyl-			100	C6H12O	000565-69-5	45



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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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	3.189	1.1	ug/L	109983	1	6.247	522801	5.0
Propanal, 2,2-d...	4.436	1.4	ug/L	149071	1	6.247	522801	5.0
2-Butanone, 3,3...	7.163	0.6	ug/L	59663	1	6.247	522801	5.0