

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052021\
 Data File : VU043862.D
 Acq On : 20 May 2021 14:02
 Operator : SY/MD
 Sample : M2475-14
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 GB411

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\SFAMUTR051521WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU043862.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.588	69	77	93	rBV2	157314	243292	33.61%	3.815%
2	1.697	104	111	119	rVB2	4679	7398	1.02%	0.116%
3	1.919	171	180	191	rVB	56646	73345	10.13%	1.150%
4	2.572	370	383	397	rBV	131622	213022	29.43%	3.341%
5	2.658	398	410	442	rVB	14275	46844	6.47%	0.735%
6	2.800	442	454	468	rBV	54650	93775	12.95%	1.471%
7	3.253	564	595	597	rBV4	15632	55674	7.69%	0.873%
8	4.449	950	967	986	rBV2	22807	61645	8.52%	0.967%
9	4.649	1012	1029	1075	rBV2	89212	309275	42.72%	4.850%
10	5.076	1143	1162	1187	rBV3	117446	296945	41.02%	4.657%
11	5.735	1346	1367	1389	rBV2	234495	604776	83.54%	9.484%
12	6.256	1514	1529	1554	rBV	293462	554844	76.64%	8.701%
13	6.700	1652	1667	1685	rBV	145854	287790	39.75%	4.513%
14	7.137	1790	1803	1807	rBV4	12159	23232	3.21%	0.364%
15	7.176	1807	1815	1842	rVB2	36276	76829	10.61%	1.205%
16	7.575	1926	1939	1955	rBV	69297	123725	17.09%	1.940%
17	7.906	2029	2042	2055	rBV	275227	475352	65.66%	7.455%
18	7.976	2059	2064	2075	rVB	6988	10400	1.44%	0.163%
19	8.189	2117	2130	2146	rBV	42236	72363	10.00%	1.135%
20	8.481	2209	2221	2236	rVB3	5317	11144	1.54%	0.175%
21	8.645	2259	2272	2310	rBV	323675	658085	90.90%	10.320%
22	9.423	2499	2514	2534	rBV	435625	723939	100.00%	11.353%
23	10.764	2915	2931	2948	rBV	120882	191399	26.44%	3.002%
24	10.899	2961	2973	2983	rBV2	9590	15596	2.15%	0.245%
25	11.819	3246	3259	3281	rBV	429671	679617	93.88%	10.658%
26	12.070	3328	3337	3350	rBV4	5790	10202	1.41%	0.160%
27	12.201	3361	3378	3398	rBV	275048	456149	63.01%	7.153%

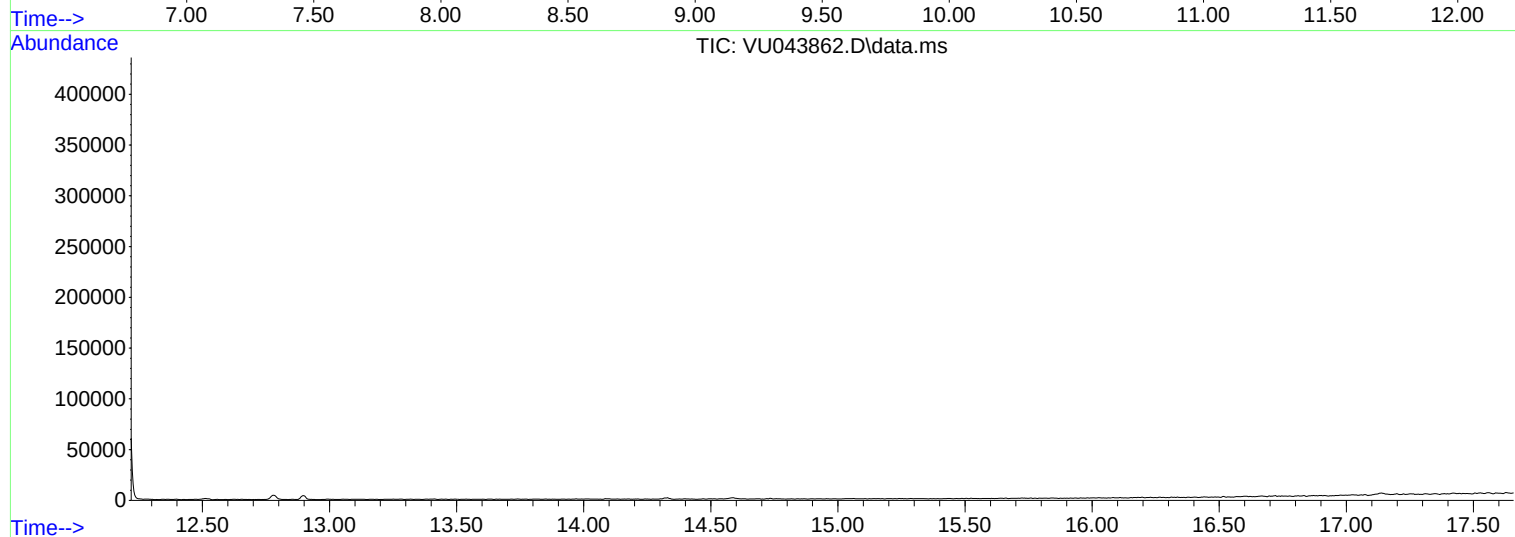
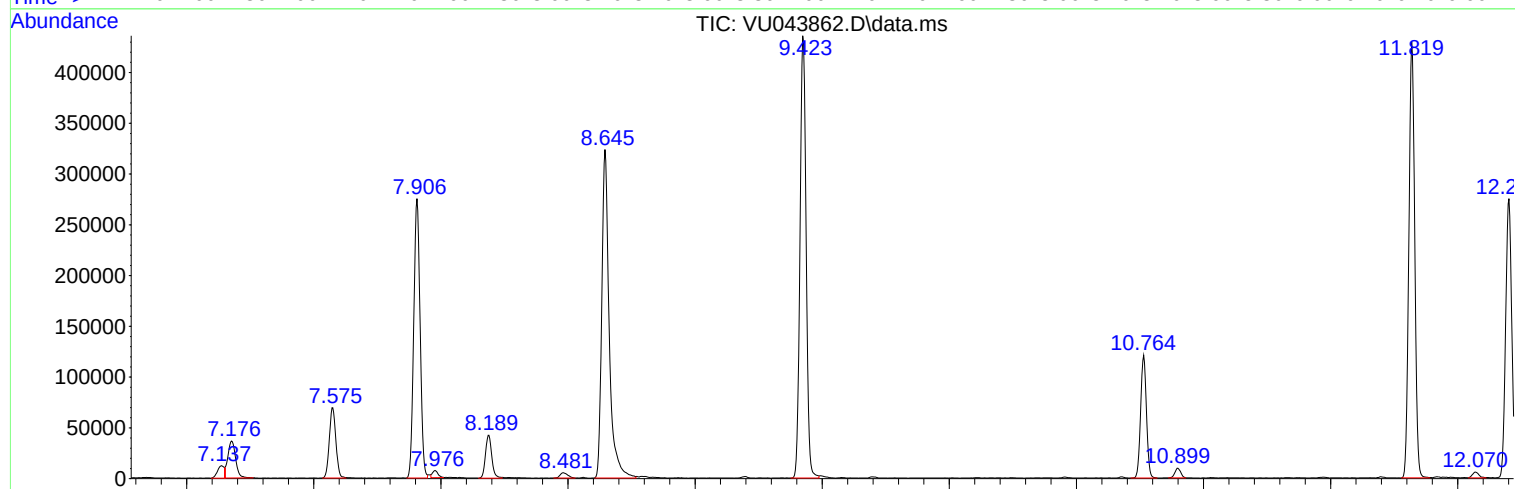
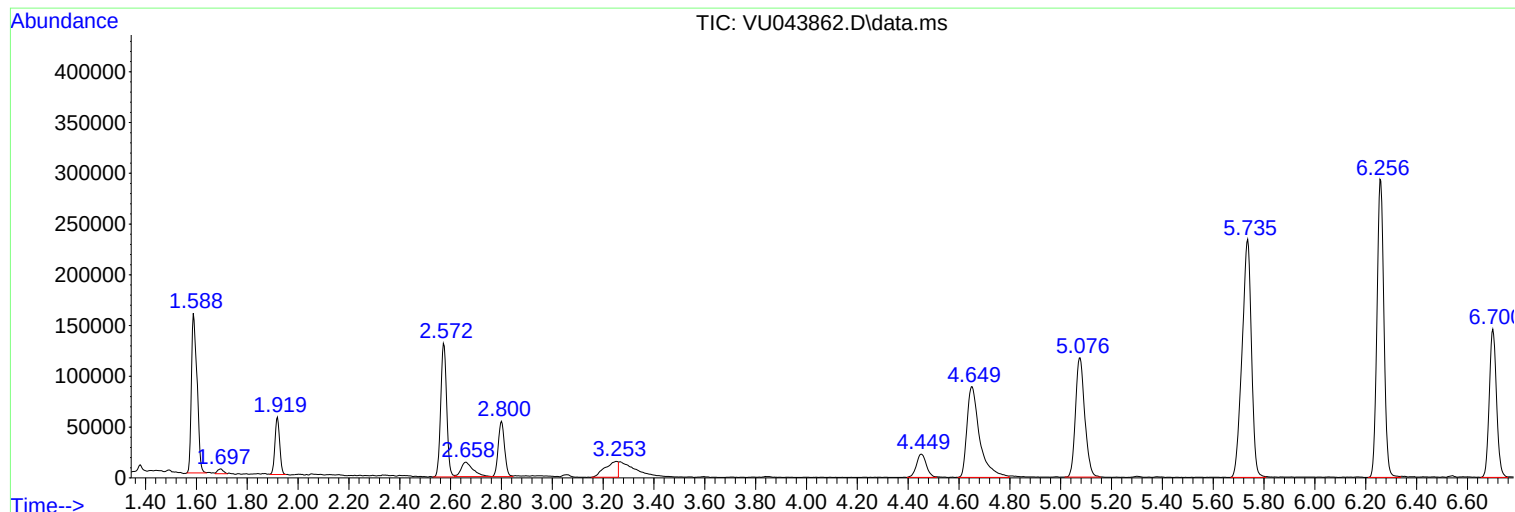
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Instrument :
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ClientSampleId :
GB411

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051521WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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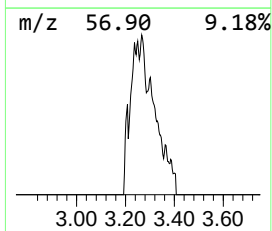
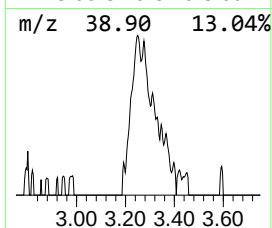
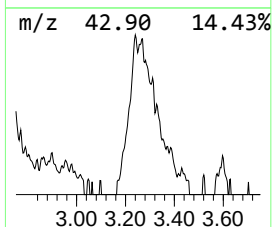
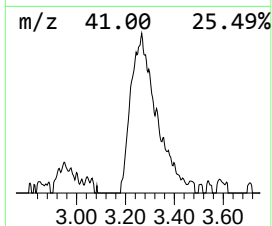
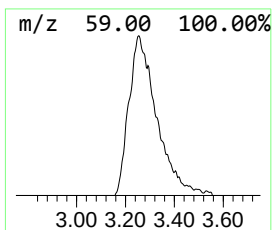
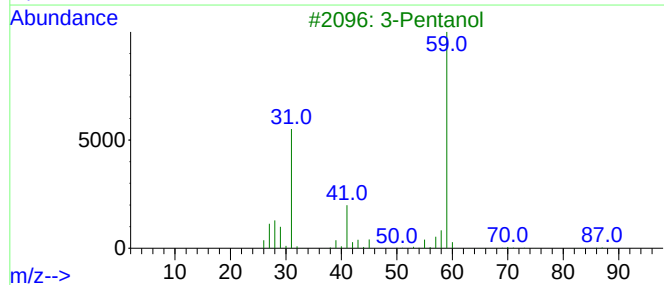
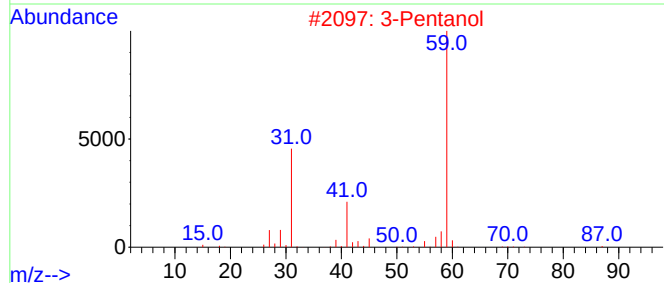
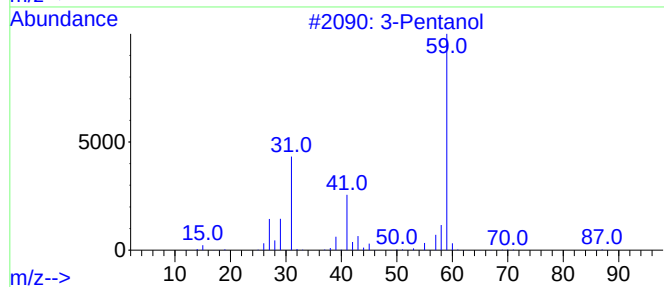
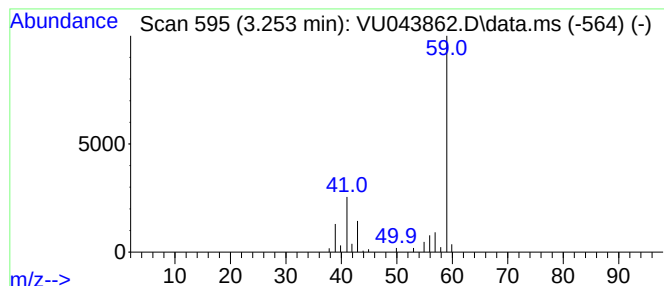
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR051521WMA.M
Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.253	0.50 ug/L	55674	1,4-Difluorobenzene	6.260

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pentanol	88	C5H12O	000584-02-1	40
2		3-Pentanol	88	C5H12O	000584-02-1	9
3		3-Pentanol	88	C5H12O	000584-02-1	9
4		Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	9
5		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	9



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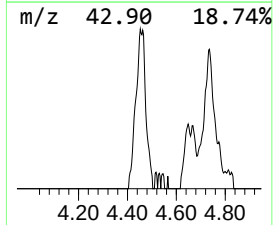
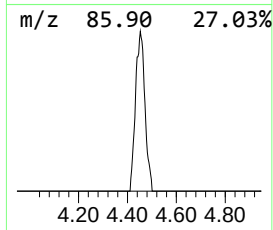
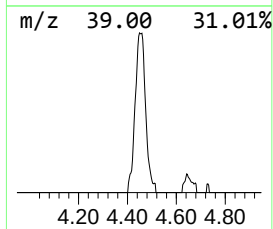
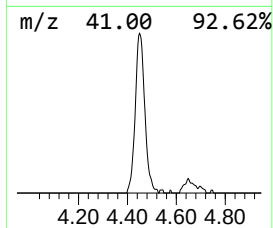
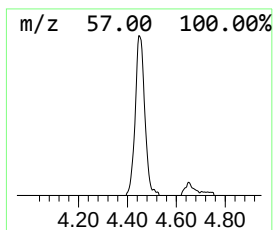
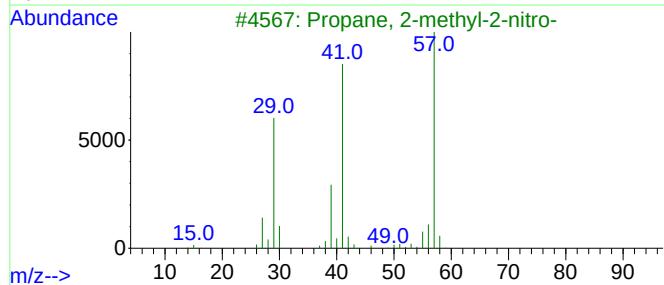
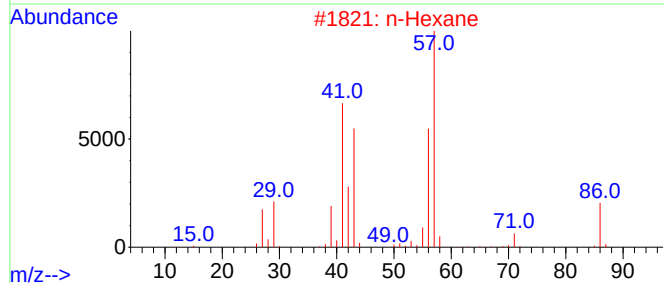
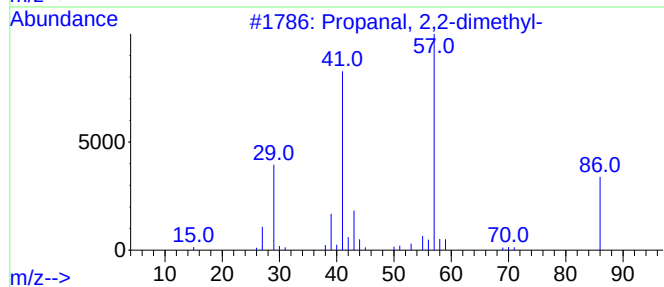
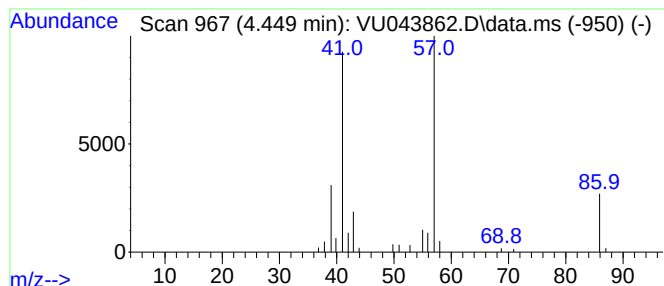
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.449	0.56 ug/L	61645	1,4-Difluorobenzene	6.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	72
2			n-Hexane	86	C6H14	000110-54-3	64
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	50
5			Butane, 2-nitro-	103	C4H9NO2	000600-24-8	40



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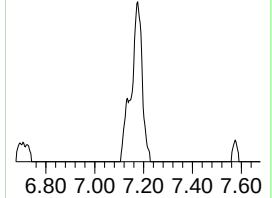
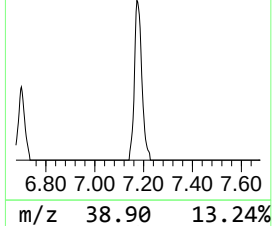
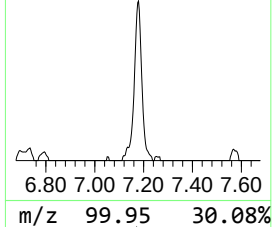
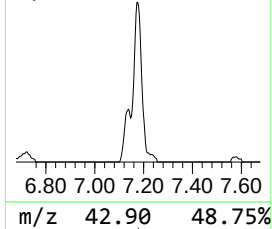
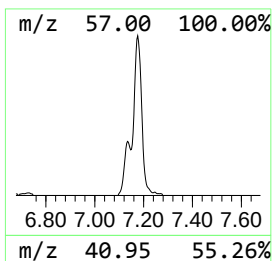
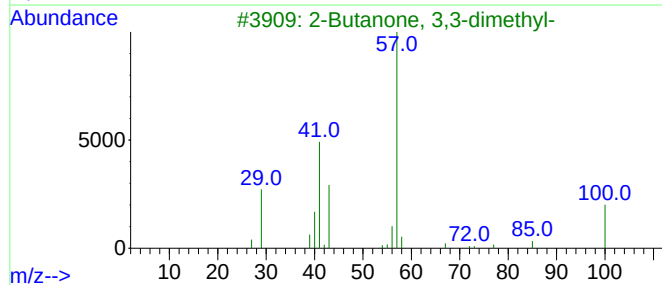
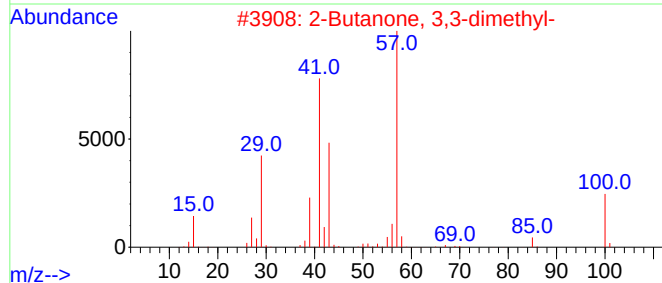
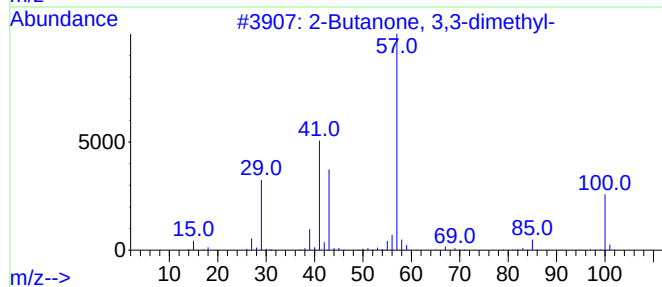
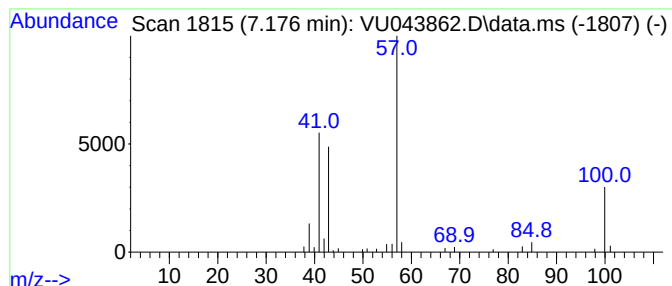
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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.176	0.69 ug/L	76829	1,4-Difluorobenzene	6.260

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	80	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	59	
3	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	53	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	50	
5	3-Hexanone		100	C6H12O	000589-38-8	42	



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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	3.253	0.5	ug/L	55674	1	6.260	554844	5.0
Propanal, 2,2-d...	4.449	0.6	ug/L	61645	1	6.260	554844	5.0
2-Butanone, 3,3...	7.176	0.7	ug/L	76829	1	6.260	554844	5.0