

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU122623\
 Data File : VU057253.D
 Acq On : 26 Dec 2023 23:39
 Operator : MD/SY
 Sample : 05976-12
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH7X5

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON
 Sampling : 1
 Start Thrs : 0.1
 Stop Thrs : 0
 Filtering: 5
 Min Area: 3 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122123WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057253.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	84	95	109	rVB2	131592	190654	27.81%	3.292%
2	1.692	116	125	146	rBV	41372	81374	11.87%	1.405%
3	1.911	185	193	211	rVB	87607	122494	17.87%	2.115%
4	2.563	384	396	411	rVB	180005	294396	42.94%	5.083%
5	2.663	414	427	433	rBV4	8395	19956	2.91%	0.345%
6	3.178	577	587	602	rVB2	5917	12203	1.78%	0.211%
7	4.438	960	979	994	rBV7	6771	19954	2.91%	0.345%
8	4.644	1028	1043	1084	rBV	47940	211413	30.83%	3.650%
9	5.055	1155	1171	1196	rBV	144682	343414	50.08%	5.929%
10	5.721	1357	1378	1402	rBV2	257592	685664	100.00%	11.839%
11	6.245	1528	1541	1558	rBV	181441	354211	51.66%	6.116%
12	6.685	1664	1678	1697	rBV	157478	311904	45.49%	5.385%
13	6.775	1700	1706	1725	rVB4	6295	14875	2.17%	0.257%
14	6.882	1730	1739	1756	rVB3	8576	16394	2.39%	0.283%
15	7.563	1939	1951	1976	rBV2	72364	132583	19.34%	2.289%
16	7.894	2041	2054	2067	rBV	287061	503757	73.47%	8.698%
17	7.965	2067	2076	2099	rVB2	57228	102769	14.99%	1.774%
18	8.177	2129	2142	2162	rBV2	45089	79721	11.63%	1.376%
19	8.470	2225	2233	2244	rBV3	7842	13760	2.01%	0.238%
20	8.634	2271	2284	2314	rBV2	242431	542690	79.15%	9.370%
21	8.785	2322	2331	2351	rVB3	33349	60170	8.78%	1.039%
22	9.412	2514	2526	2544	rBV	262175	459110	66.96%	7.927%
23	9.570	2565	2575	2585	rBV	8211	14910	2.17%	0.257%
24	9.689	2600	2612	2625	rBV	26271	47094	6.87%	0.813%
25	10.097	2729	2739	2749	rBV2	10251	17213	2.51%	0.297%
26	10.235	2772	2782	2799	rBV	31319	53742	7.84%	0.928%
27	10.753	2931	2943	2959	rBV2	108638	181334	26.45%	3.131%
28	10.891	2976	2986	2998	rVB3	16929	27244	3.97%	0.470%
29	11.573	3189	3198	3211	rVB6	5336	8692	1.27%	0.150%
30	11.807	3258	3271	3290	rBV	257794	417565	60.90%	7.210%
31	12.190	3377	3390	3409	rBV	254066	426062	62.14%	7.356%
32	12.891	3599	3608	3618	rBV5	5365	8288	1.21%	0.143%
33	14.569	4115	4130	4141	rBV2	9861	16158	2.36%	0.279%

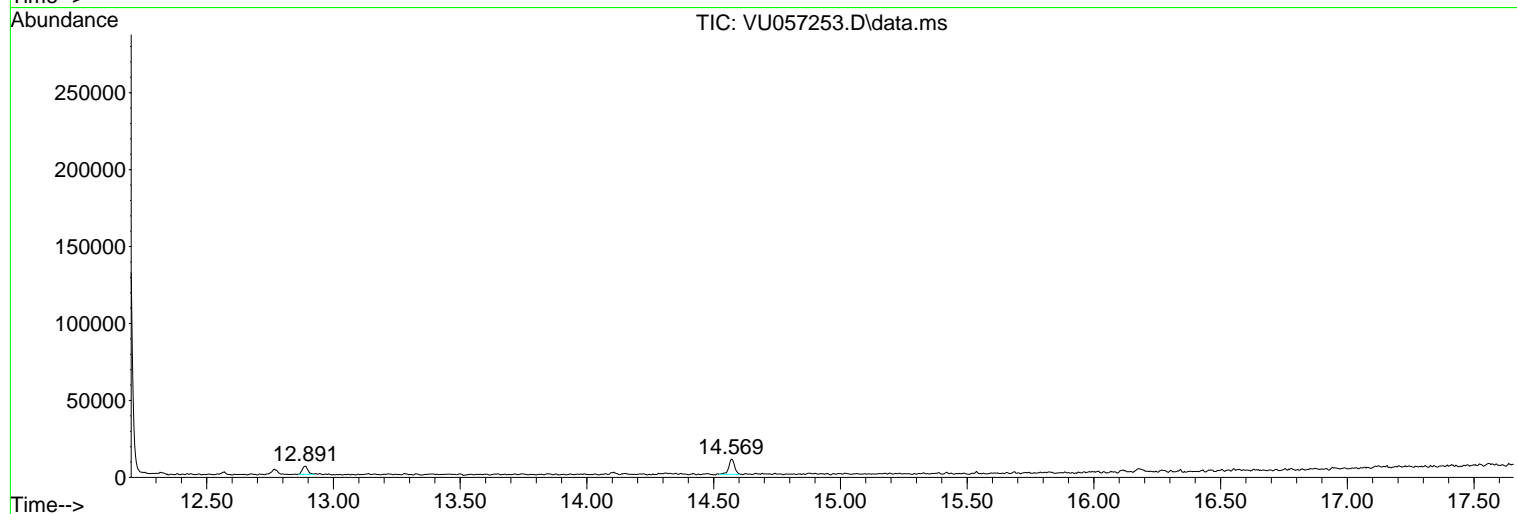
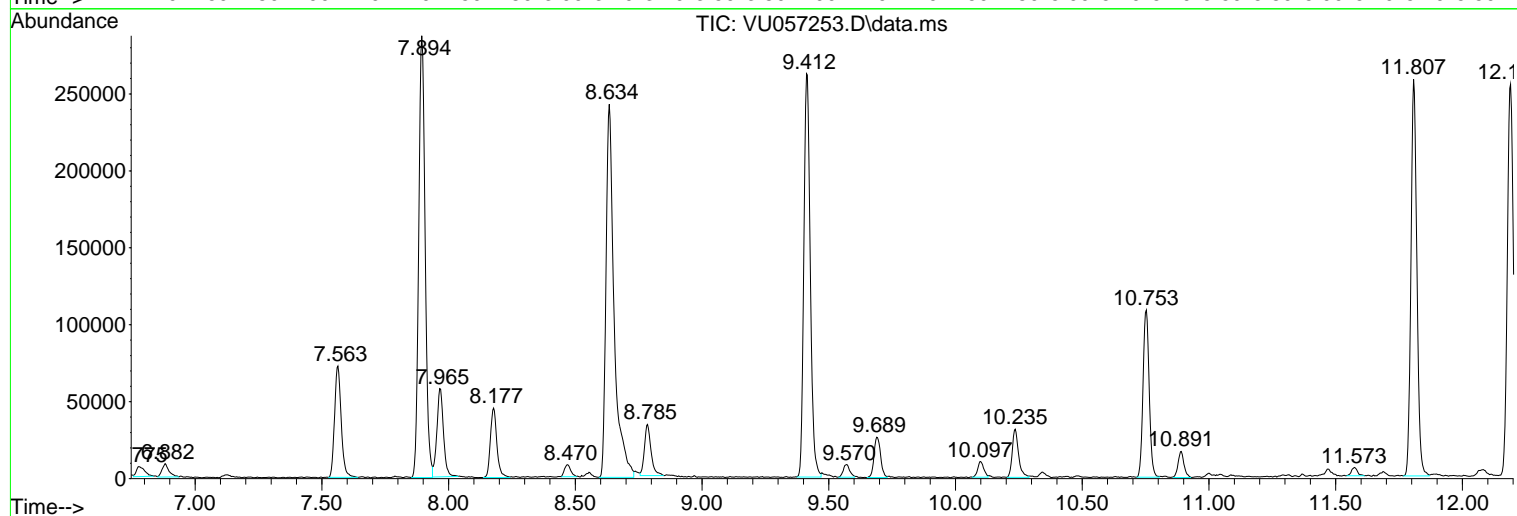
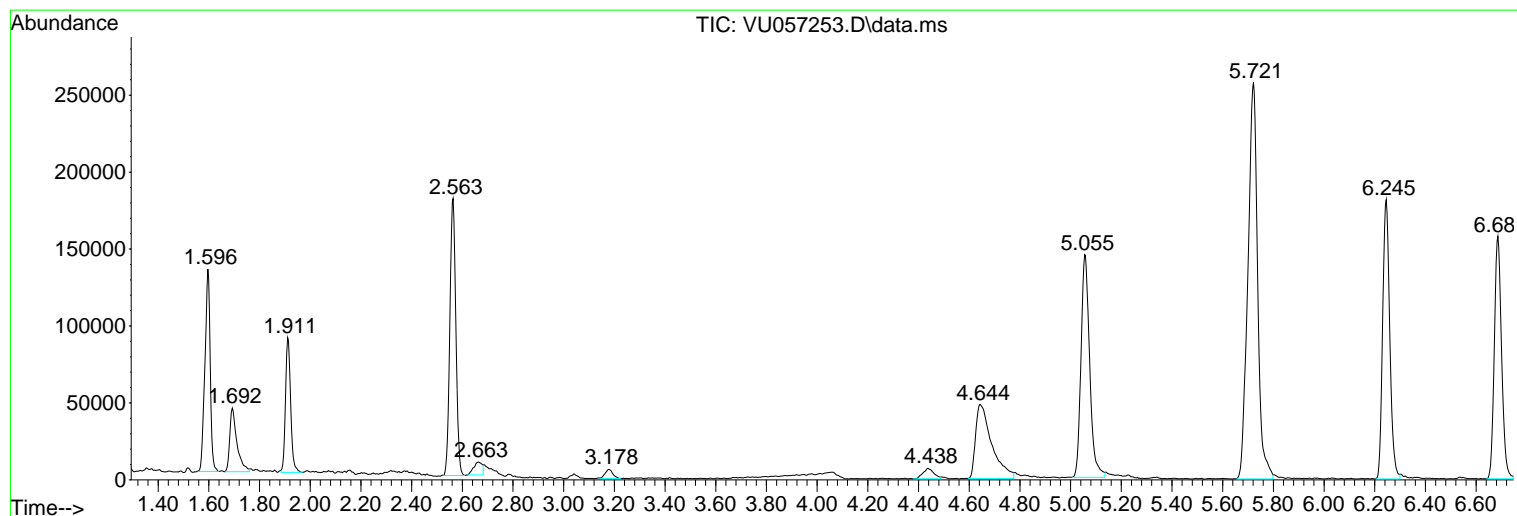
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122123WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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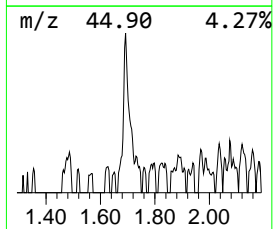
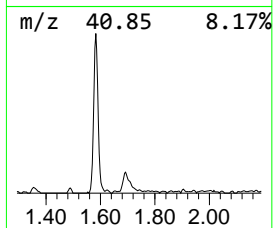
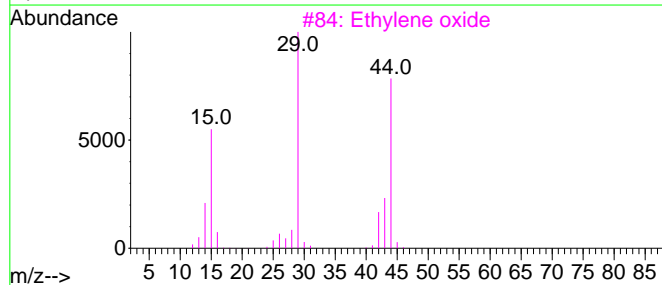
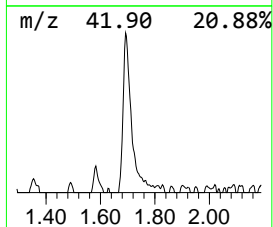
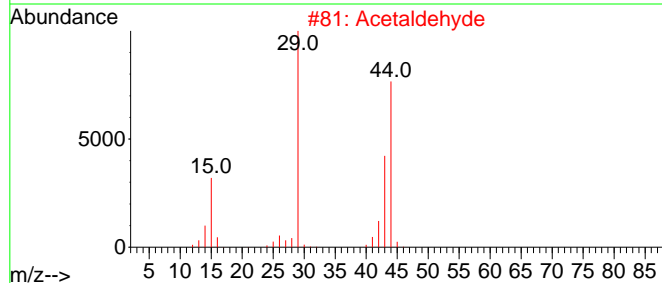
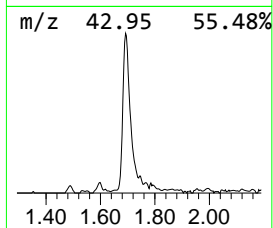
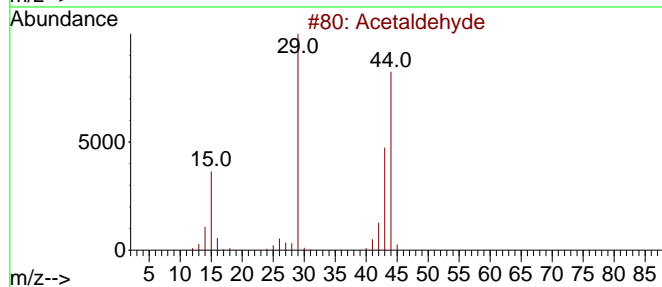
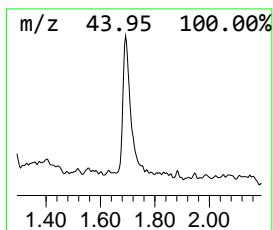
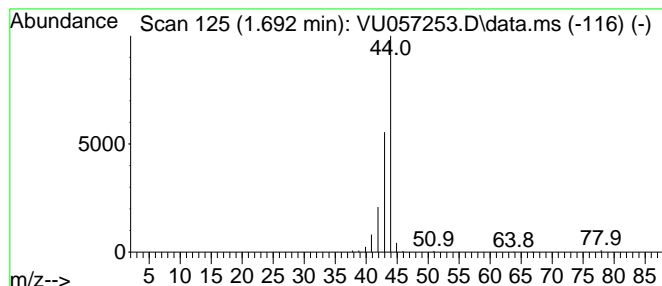
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122123WMA.M
 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.692	1.15 ug/L	81374	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	74
2			Acetaldehyde	44	C2H4O	000075-07-0	74
3			Ethylene oxide	44	C2H4O	000075-21-8	9
4			Ethylene oxide	44	C2H4O	000075-21-8	5
5			Ethylene oxide	44	C2H4O	000075-21-8	5



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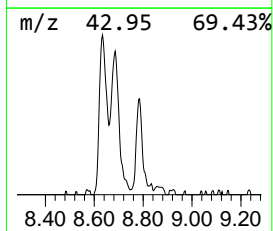
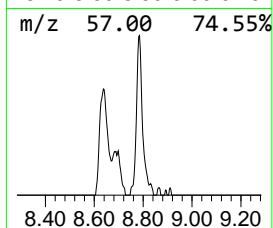
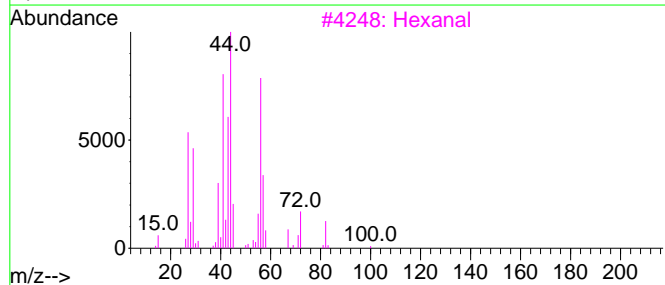
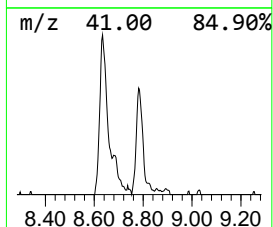
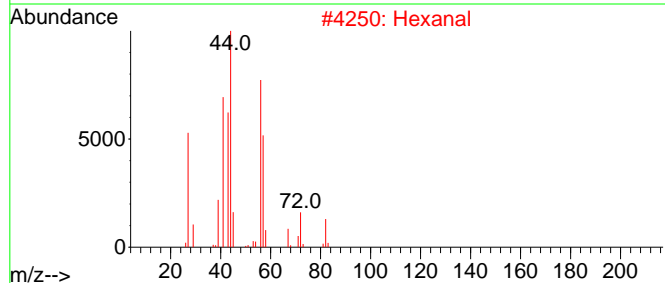
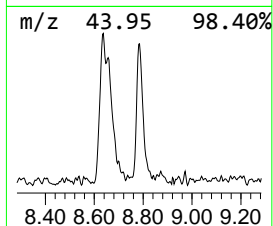
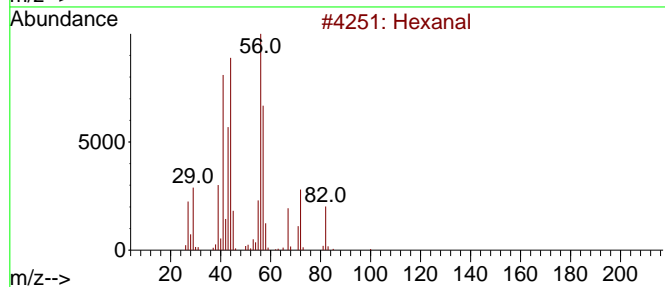
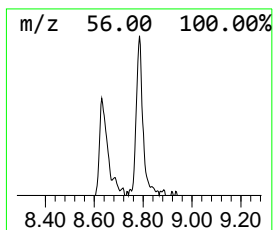
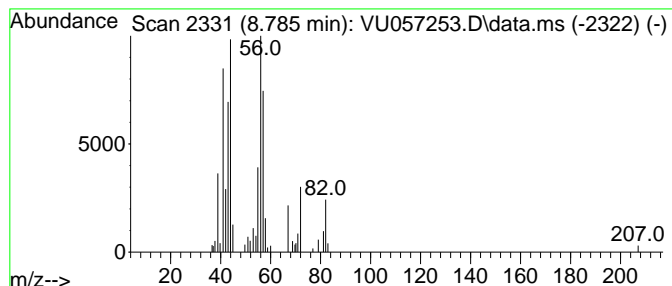
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR122123WMA.M
 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 3 Hexanal Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	0.66 ug/L	60170	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal	100	C6H12O	000066-25-1	64
2			Hexanal	100	C6H12O	000066-25-1	59
3			Hexanal	100	C6H12O	000066-25-1	50
4			1-Cyclopropylguanidine	99	C4H9N3	168627-33-6	42
5			Glutaraldehyde	100	C5H8O2	000111-30-8	38



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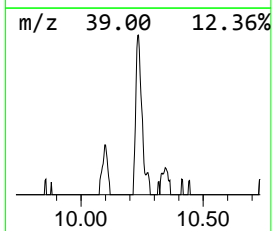
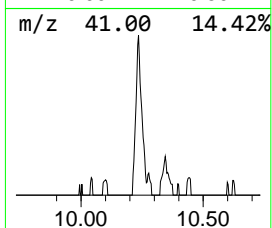
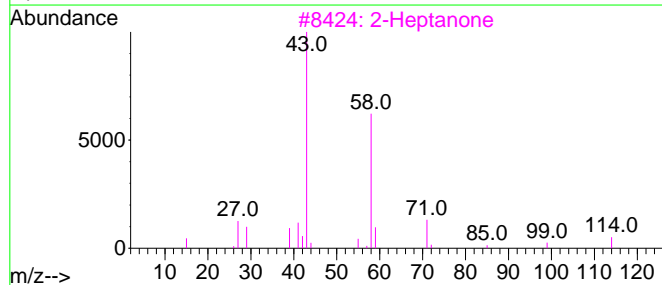
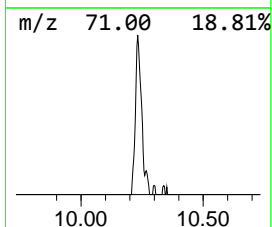
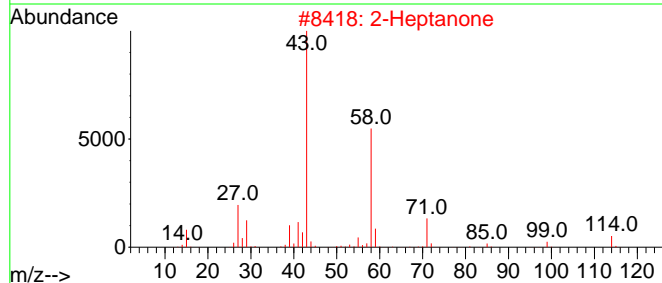
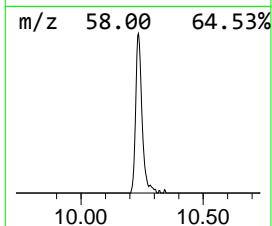
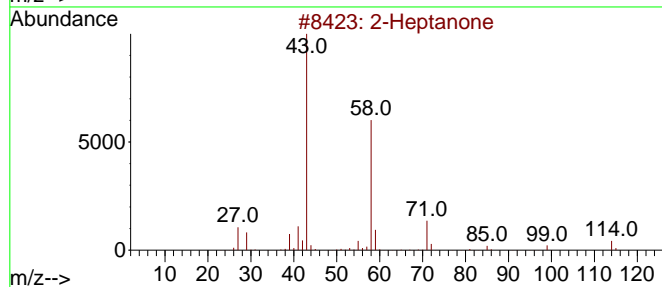
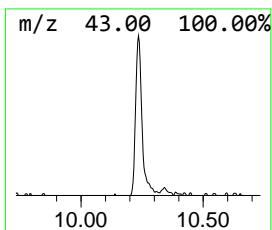
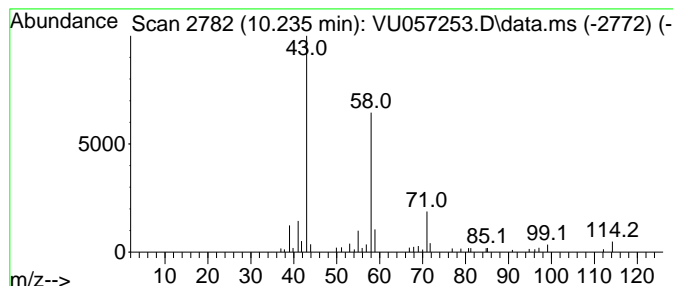
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 Quant Title : TRACE VOA SFAM1.0

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

 Peak Number 4 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.235	0.59 ug/L	53742	Chlorobenzene-d5	9.415

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Heptanone	114	C7H14O	000110-43-0	91
2			2-Heptanone	114	C7H14O	000110-43-0	86
3			2-Heptanone	114	C7H14O	000110-43-0	86
4			2-Heptanone	114	C7H14O	000110-43-0	83
5			2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78



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Quant Title : TRACE VOA SFAM1.0

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.692	1.1	ug/L	81374	1	6.245	354211	5.0
Hexanal	8.785	0.7	ug/L	60170	2	9.415	459110	5.0
2-Heptanone	10.235	0.6	ug/L	53742	2	9.415	459110	5.0