

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
 Data File : VU059513.D
 Acq On : 26 Jun 2024 09:41
 Operator : MD/SY
 Sample : P2962-01
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 63 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0T73

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\SFAMUTR061724WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU059513.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	rBV2	59929	88401	17.20%	1.875%
2	1.682	113	122	145	rBV	110335	150491	29.28%	3.191%
3	1.907	184	192	207	rVB	53421	73888	14.38%	1.567%
4	2.329	312	323	335	rBV2	7534	12914	2.51%	0.274%
5	2.560	379	395	406	rBV2	97871	162293	31.58%	3.442%
6	2.628	406	416	455	rVB	71347	154967	30.15%	3.286%
7	3.036	536	543	558	rVB4	2996	5865	1.14%	0.124%
8	3.200	579	594	618	rBV4	5325	16863	3.28%	0.358%
9	4.438	958	979	998	rBV7	16515	52497	10.21%	1.113%
10	4.621	1024	1036	1058	rBV	70731	189427	36.86%	4.017%
11	5.055	1155	1171	1200	rVB	100132	220810	42.96%	4.683%
12	5.718	1358	1377	1406	rBV2	189752	496552	96.62%	10.530%
13	6.242	1524	1540	1571	rBV	157523	317868	61.85%	6.741%
14	6.682	1664	1677	1701	rBV	118964	235068	45.74%	4.985%
15	6.779	1701	1707	1718	rVB4	2791	5515	1.07%	0.117%
16	6.881	1732	1739	1750	rBV4	4956	10589	2.06%	0.225%
17	7.123	1802	1814	1819	rBV3	4160	7333	1.43%	0.156%
18	7.563	1939	1951	1972	rBV2	48207	89136	17.34%	1.890%
19	7.894	2041	2054	2072	rBV	222197	395507	76.96%	8.388%
20	8.177	2131	2142	2153	rBV2	30879	53947	10.50%	1.144%
21	8.627	2271	2282	2323	rBV	244917	513940	100.00%	10.899%
22	8.785	2323	2331	2345	rVB3	16185	28090	5.47%	0.596%
23	9.412	2512	2526	2554	rBV	238040	405334	78.87%	8.596%
24	9.647	2590	2599	2611	rBV3	7077	12278	2.39%	0.260%
25	10.132	2742	2750	2761	rVB3	4161	6573	1.28%	0.139%
26	10.232	2772	2781	2800	rBV	33013	58786	11.44%	1.247%
27	10.341	2808	2815	2830	rVB6	3529	6685	1.30%	0.142%
28	10.750	2931	2942	2960	rBV	105565	167589	32.61%	3.554%
29	10.859	2965	2976	2996	rVB3	10903	22232	4.33%	0.471%
30	11.807	3259	3271	3293	rBV	224801	374962	72.96%	7.952%
31	12.068	3343	3352	3358	rBV8	4151	7916	1.54%	0.168%
32	12.187	3377	3389	3410	rBV	217949	361470	70.33%	7.666%
33	12.884	3599	3606	3618	rBV5	6103	9629	1.87%	0.204%

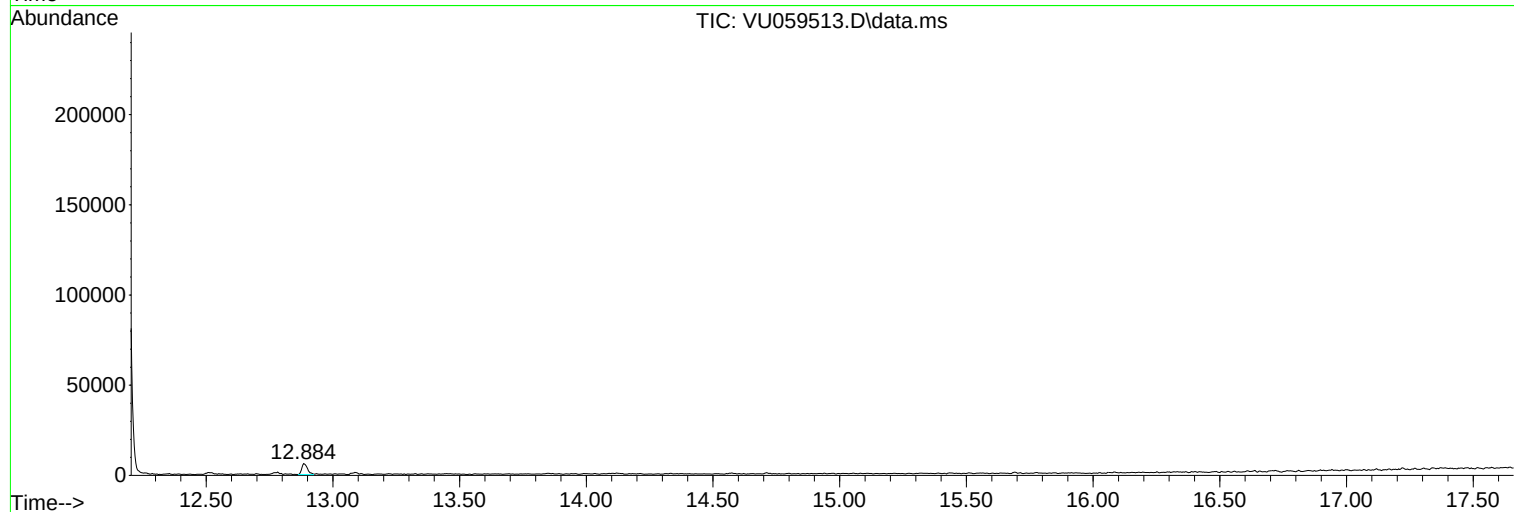
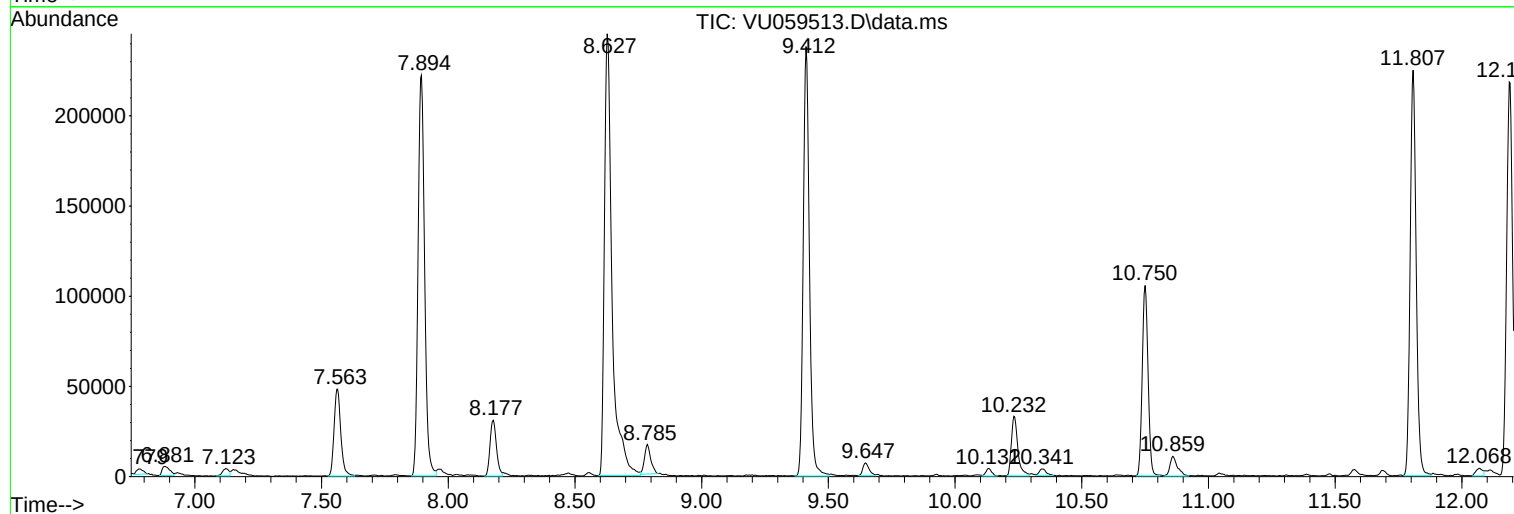
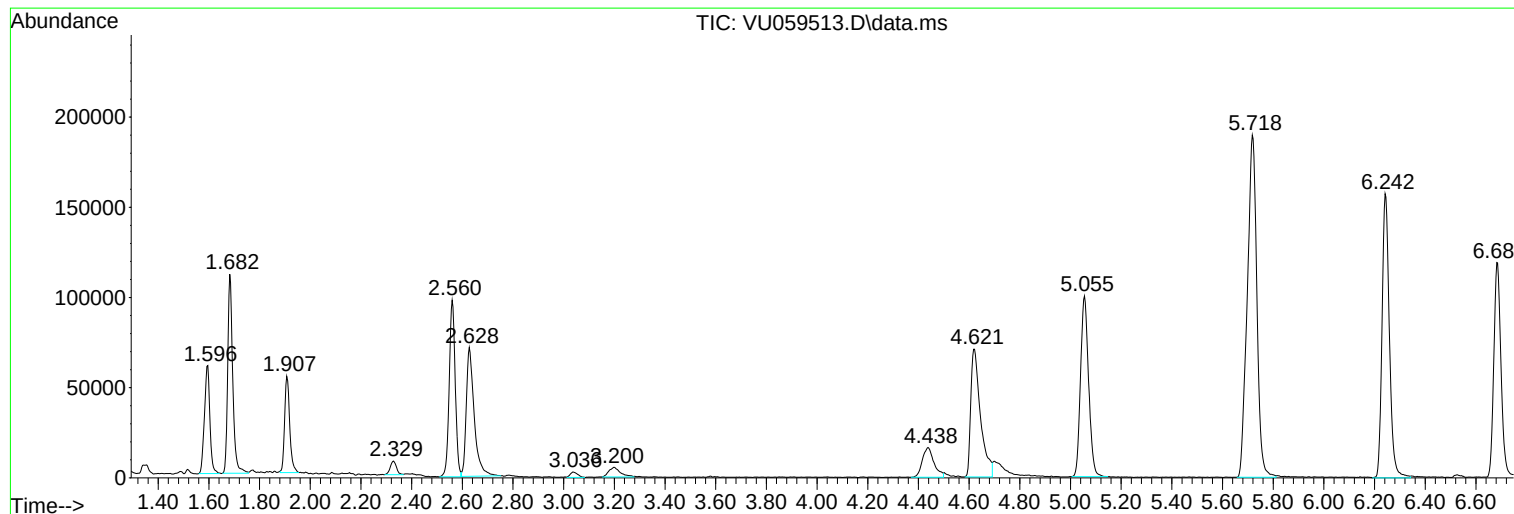
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ClientSampleId :
C0T73

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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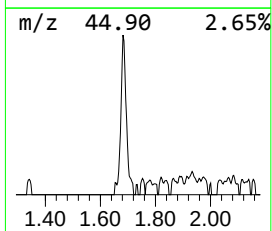
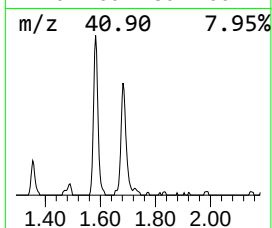
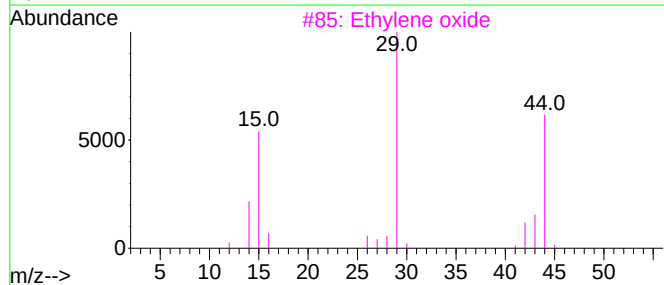
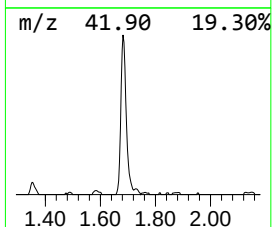
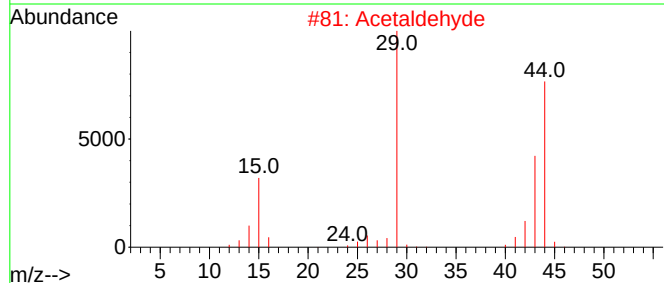
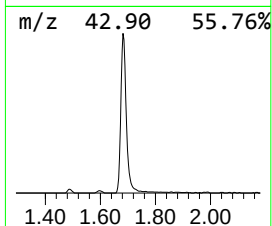
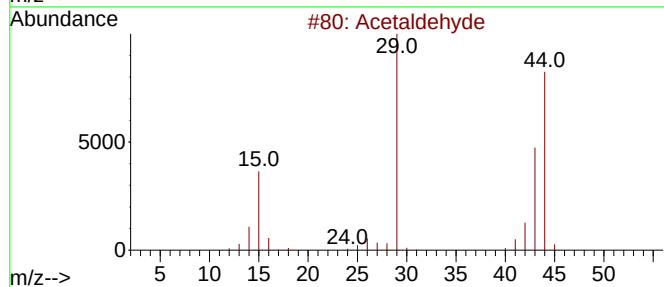
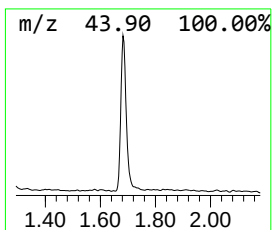
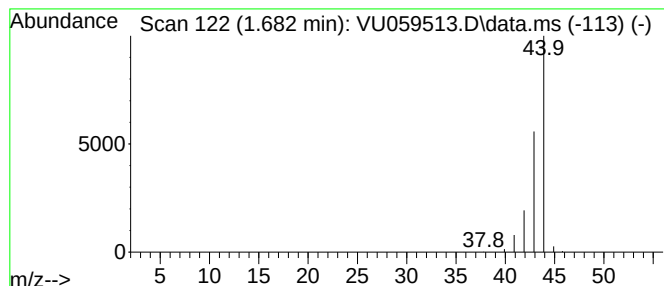
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.682	2.37 ug/L	150491	1,4-Difluorobenzene	6.245

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



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Instrument :
MSVOA_U
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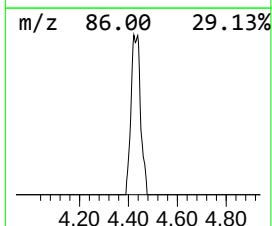
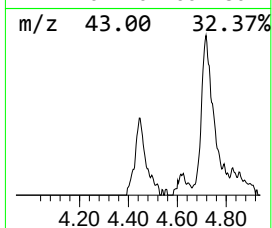
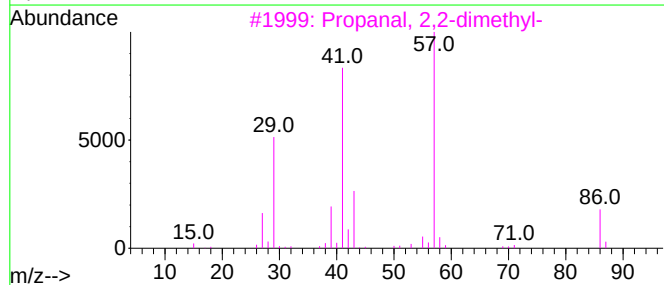
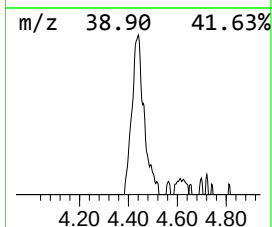
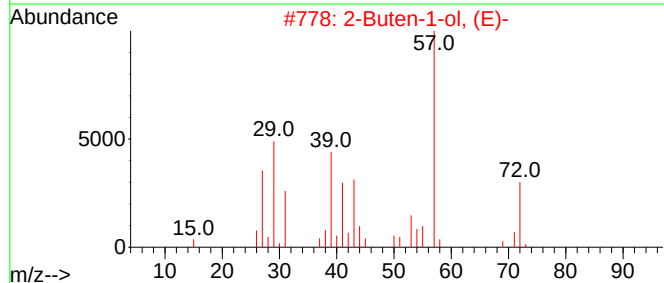
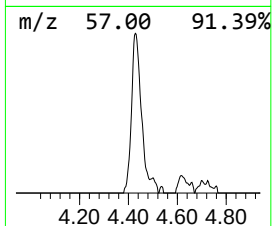
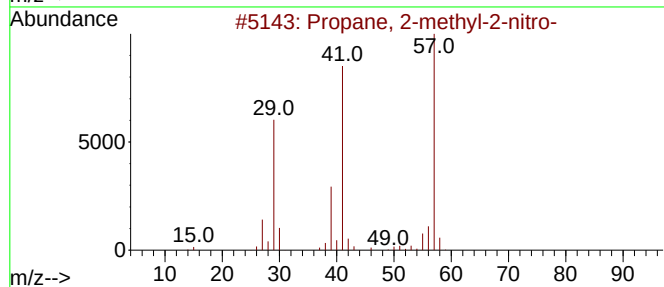
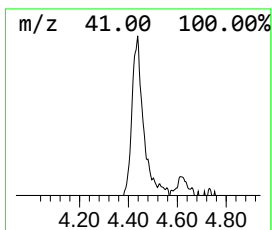
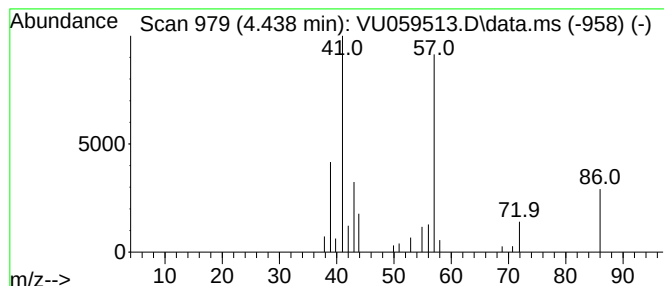
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propane, 2-methyl-2-nitro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.438	0.83 ug/L	52497	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
2			2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	38
3			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	30
4			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	30
5			Oxalic acid, allyl heptyl ester	228	C12H20O4	1000309-23-5	17



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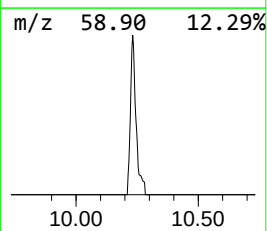
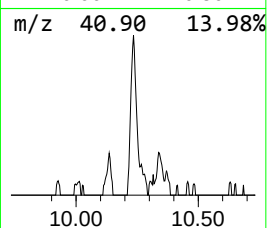
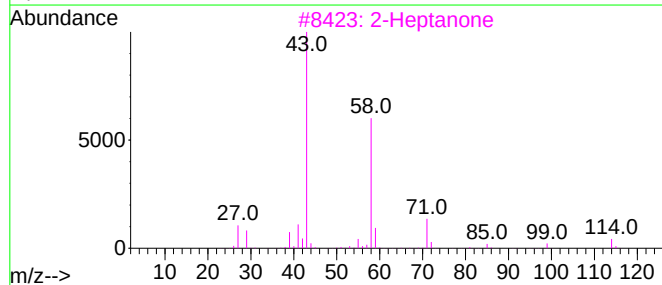
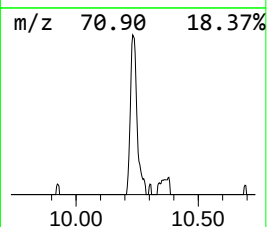
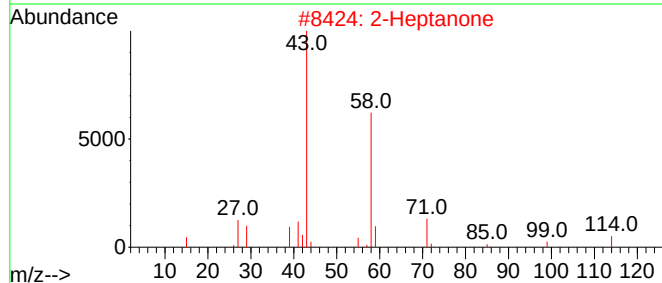
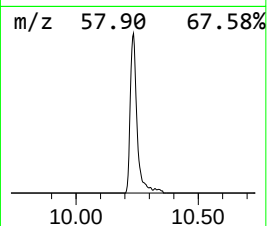
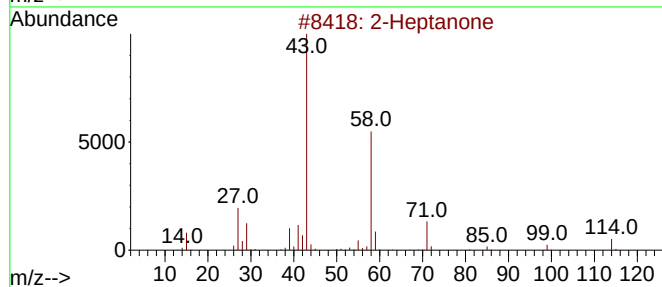
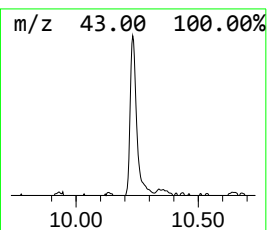
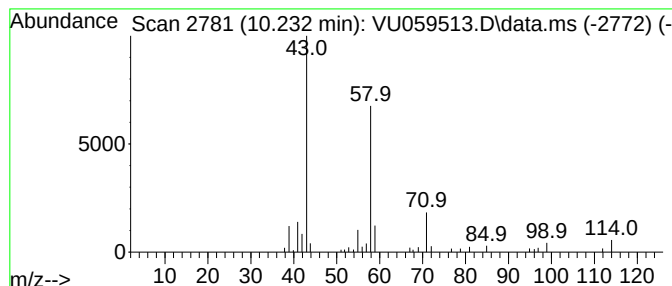
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR061724WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
10.232	0.73 ug/L	58786	Chlorobenzene-d5	9.412

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Heptanone	114	C7H14O	000110-43-0	90
2		2-Heptanone	114	C7H14O	000110-43-0	90
3		2-Heptanone	114	C7H14O	000110-43-0	87
4		2-Heptanone	114	C7H14O	000110-43-0	87
5		2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78



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ALS Vial : 63 Sample Multiplier: 1

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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
unknown-01	1.682	2.4	ug/L	150491	1	6.245	317868	5.0
Propane, 2-meth...	4.438	0.8	ug/L	52497	1	6.245	317868	5.0
2-Heptanone	10.232	0.7	ug/L	58786	2	9.412	405334	5.0