

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071824\
 Data File : VU060068.D
 Acq On : 19 Jul 2024 18:18
 Operator : MD/SY
 Sample : P3298-22
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BHB70

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\SFAMUTR071824WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU060068.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	111	rVB2	54914	83395	15.02%	1.730%
2	1.686	111	123	143	rBV	159803	247143	44.52%	5.126%
3	1.911	184	193	210	rVB	47739	66372	11.96%	1.377%
4	2.560	379	395	408	rBV	81817	136564	24.60%	2.832%
5	2.641	408	420	457	rVV	75054	217864	39.25%	4.518%
6	3.184	574	589	591	rBV2	4213	7253	1.31%	0.150%
7	4.435	960	978	1008	rBV5	37395	117979	21.25%	2.447%
8	4.628	1024	1038	1062	rBV	76848	235554	42.43%	4.885%
9	4.814	1089	1096	1112	rVB2	5243	12491	2.25%	0.259%
10	5.055	1156	1171	1201	rBV	105743	242730	43.73%	5.034%
11	5.718	1359	1377	1411	rBV2	177984	468425	84.38%	9.715%
12	6.242	1528	1540	1571	rBV	140862	277502	49.99%	5.755%
13	6.685	1665	1678	1701	rBV	111602	224012	40.35%	4.646%
14	6.785	1701	1709	1721	rVB3	3640	7625	1.37%	0.158%
15	6.882	1731	1739	1751	rBV4	6793	13941	2.51%	0.289%
16	7.123	1802	1814	1821	rBV3	11578	23654	4.26%	0.491%
17	7.560	1939	1950	1966	rBV2	51237	91431	16.47%	1.896%
18	7.894	2041	2054	2072	rBV	200189	354632	63.89%	7.355%
19	8.177	2131	2142	2159	rBV	31767	55204	9.94%	1.145%
20	8.627	2271	2282	2318	rBV	271010	555107	100.00%	11.513%
21	8.782	2322	2330	2353	rVB2	19401	36331	6.54%	0.753%
22	9.412	2514	2526	2564	rBV	208148	352907	63.57%	7.319%
23	9.647	2590	2599	2608	rBV4	4832	7973	1.44%	0.165%
24	10.232	2771	2781	2804	rBV2	32998	59967	10.80%	1.244%
25	10.750	2929	2942	2959	rBV	105590	170937	30.79%	3.545%
26	10.888	2965	2985	3000	rVB4	11152	25670	4.62%	0.532%
27	11.807	3260	3271	3290	rBV	200916	329937	59.44%	6.843%
28	12.068	3342	3352	3360	rBV5	8381	16490	2.97%	0.342%
29	12.187	3377	3389	3407	rBV	208297	345771	62.29%	7.171%
30	12.528	3487	3495	3509	rVB7	4273	6855	1.23%	0.142%
31	12.772	3559	3571	3584	rBV4	7954	13766	2.48%	0.286%
32	12.888	3598	3607	3618	rBV6	5663	8805	1.59%	0.183%
33	14.573	4114	4131	4141	rBV	4460	7356	1.33%	0.153%

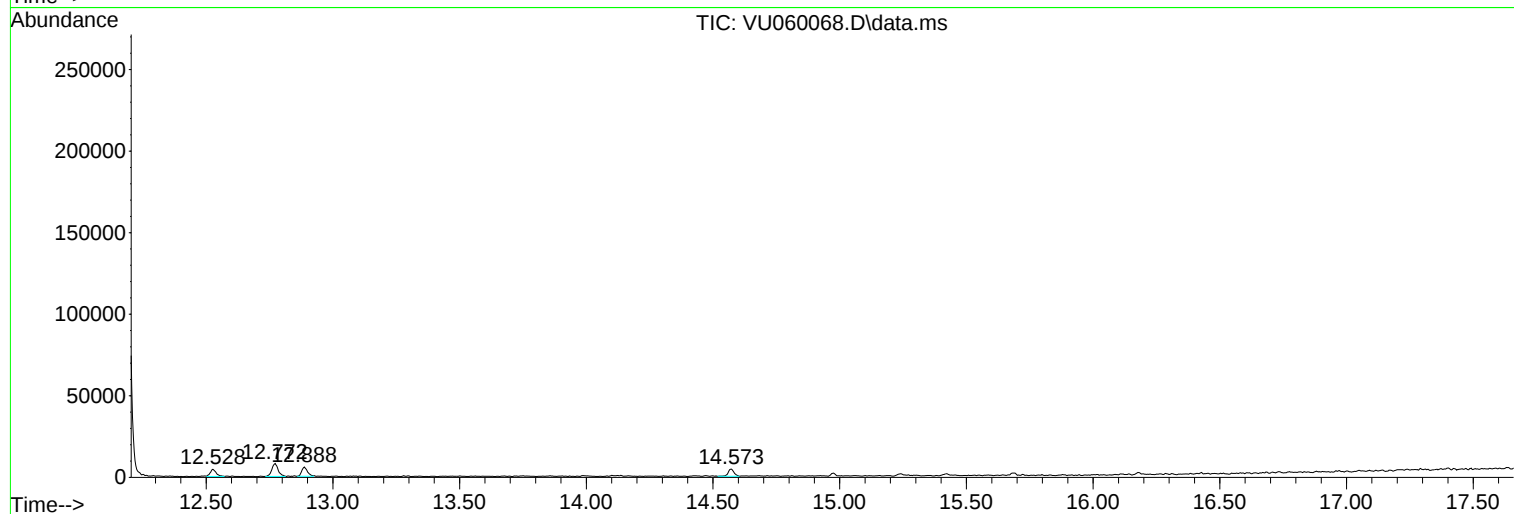
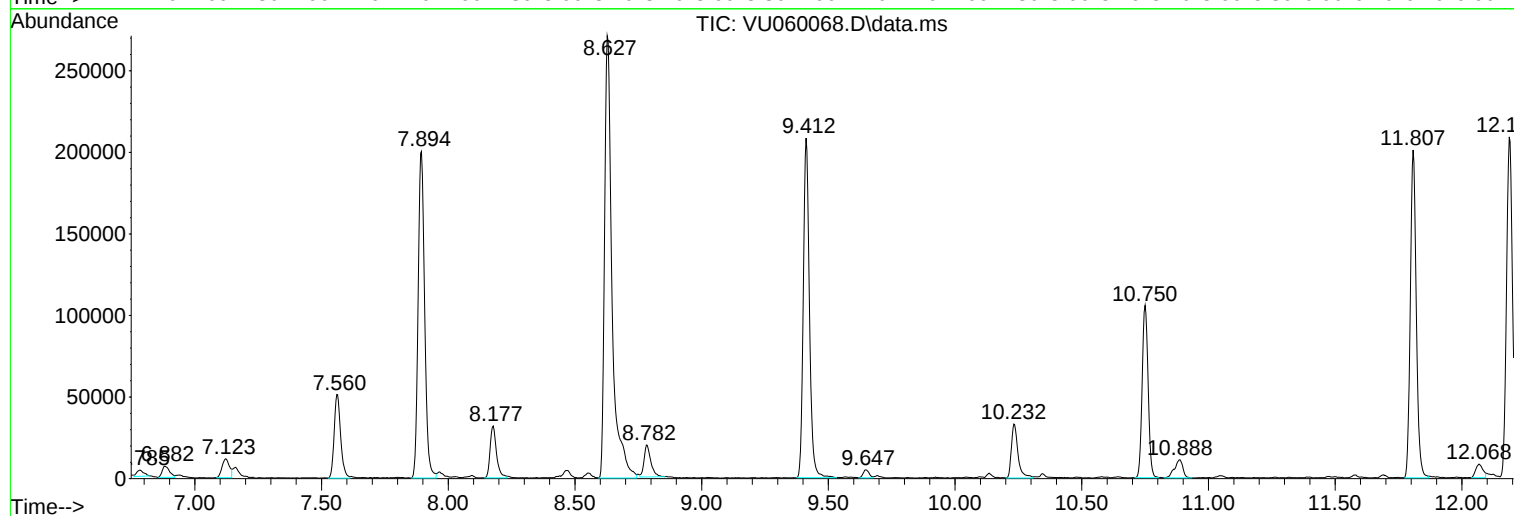
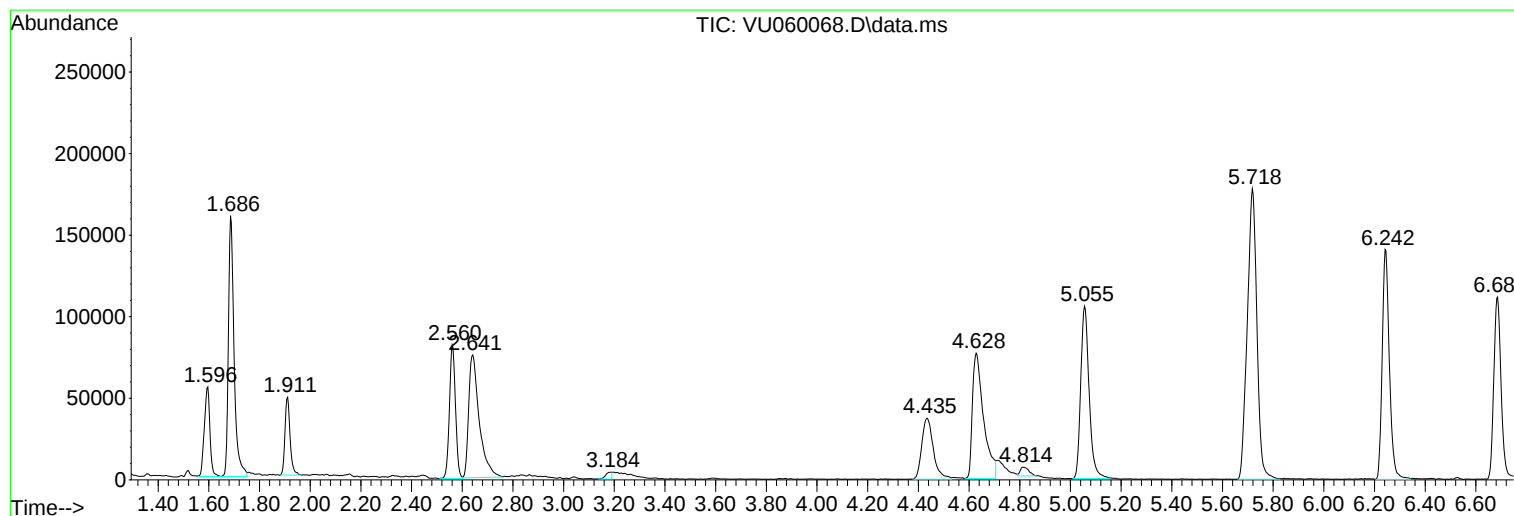
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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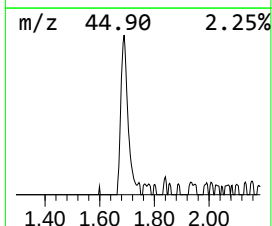
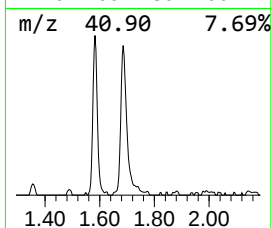
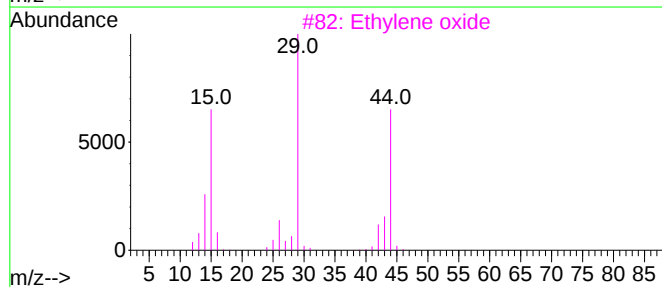
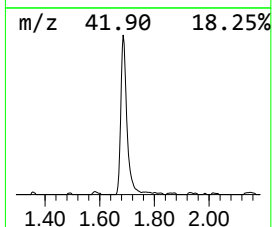
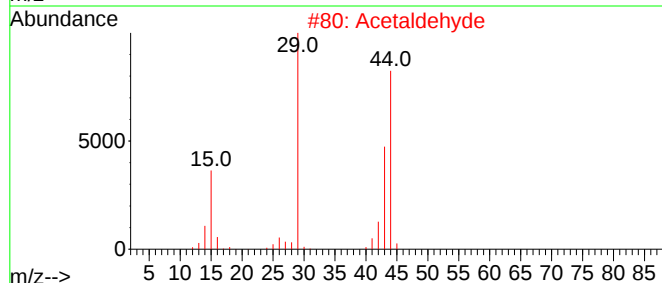
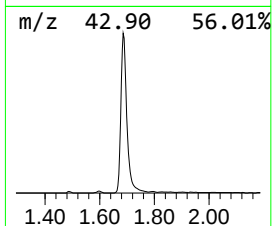
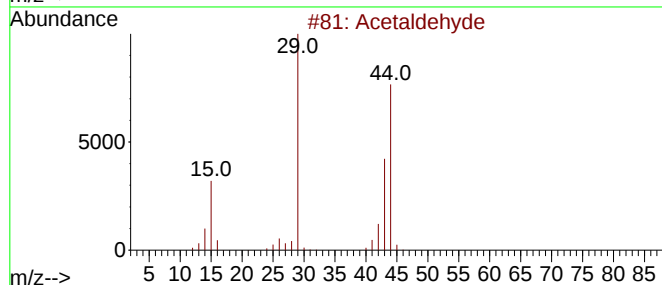
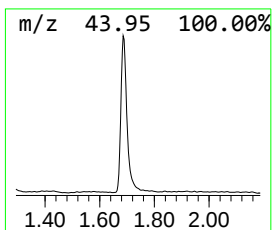
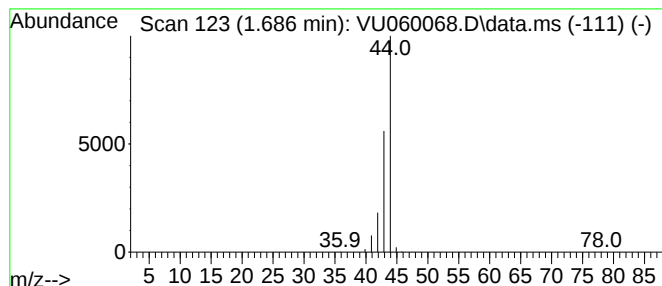
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.686	4.45 ug/L	247143	1,4-Difluorobenzene	6.242

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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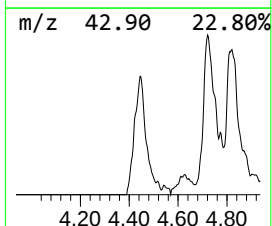
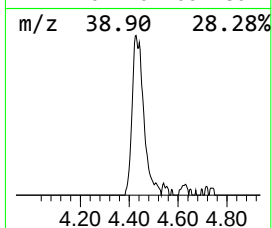
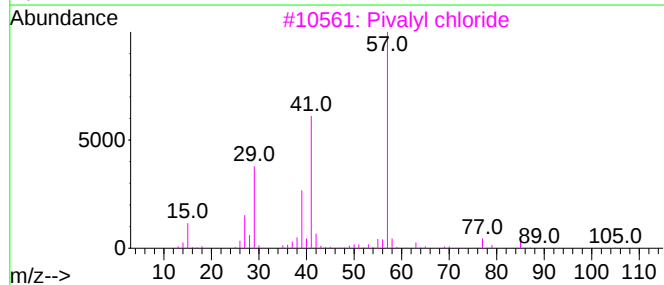
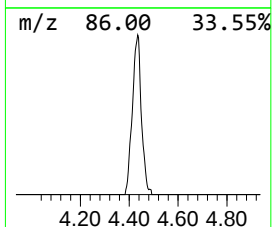
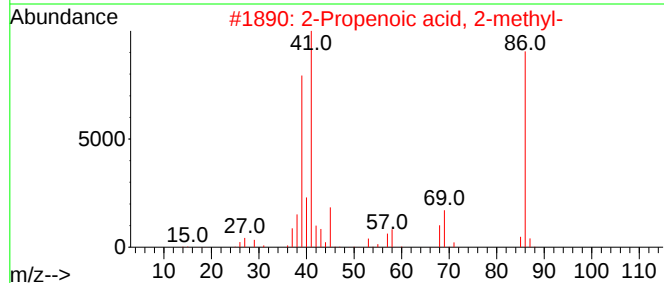
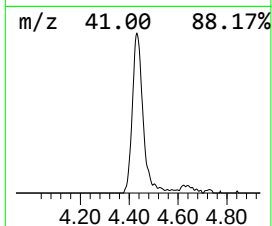
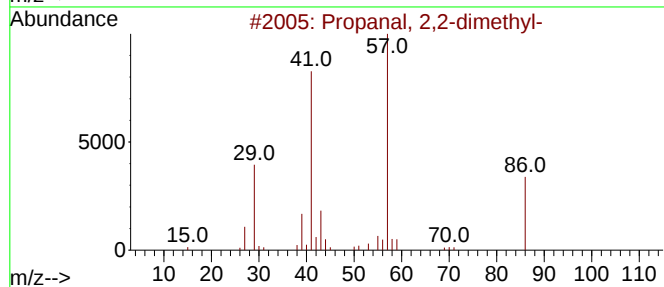
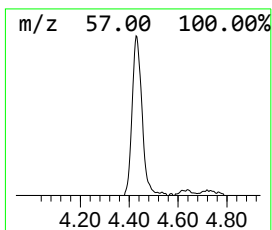
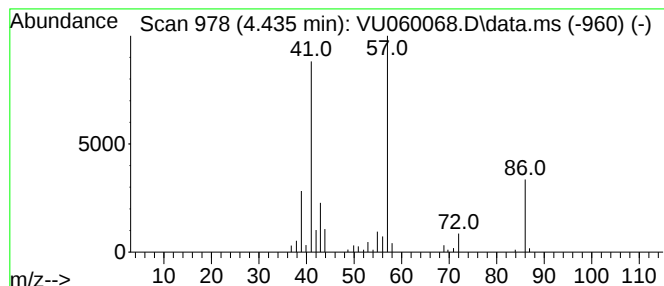
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR071824WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
4.435	2.13 ug/L	117979	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	72
2			2-Propenoic acid, 2-methyl-	86	C4H6O2	000079-41-4	50
3			Pivalyl chloride	120	C5H9ClO	003282-30-2	43
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	38
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	37



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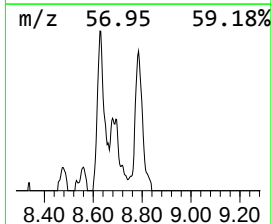
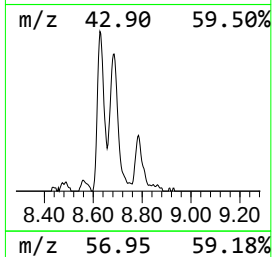
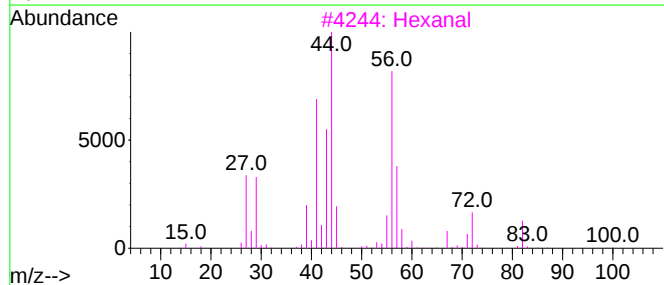
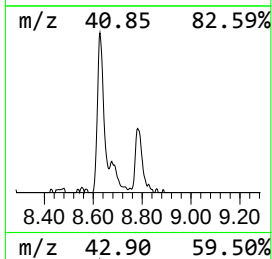
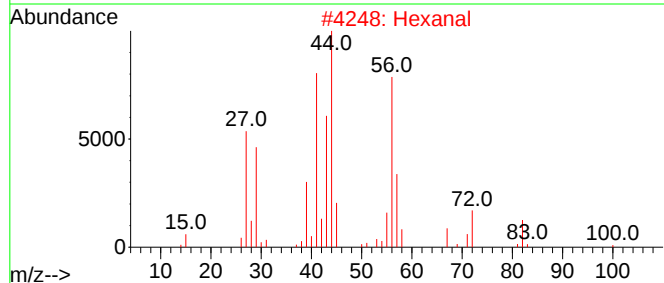
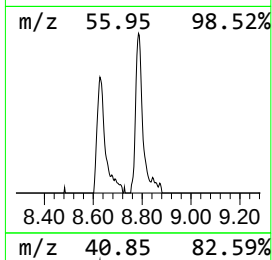
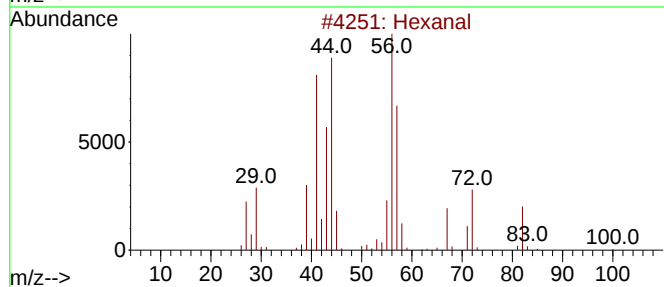
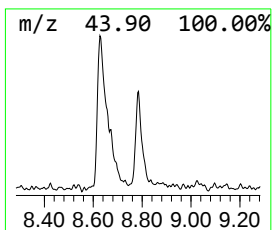
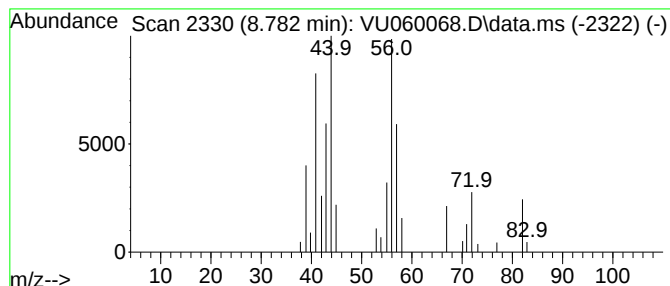
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	0.51 ug/L	36331	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	59
5	Hexanal			100	C6H12O	000066-25-1	42



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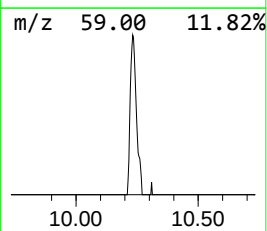
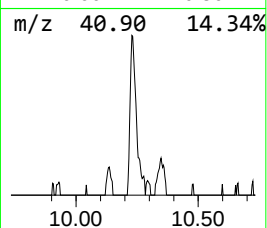
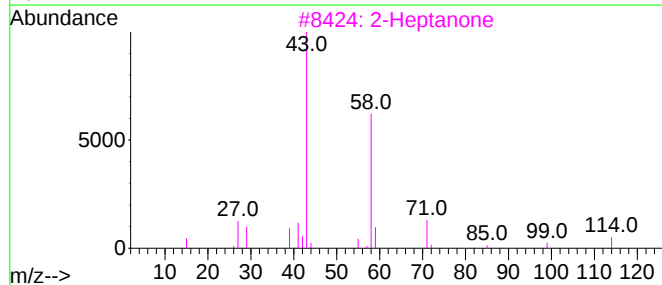
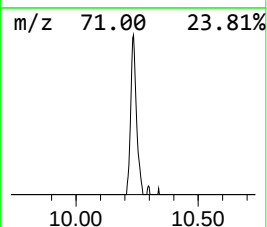
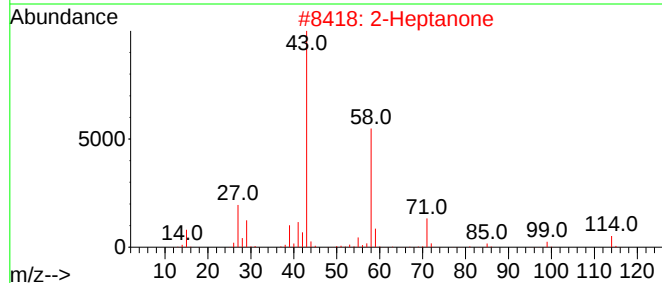
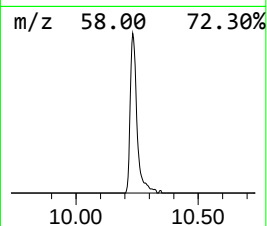
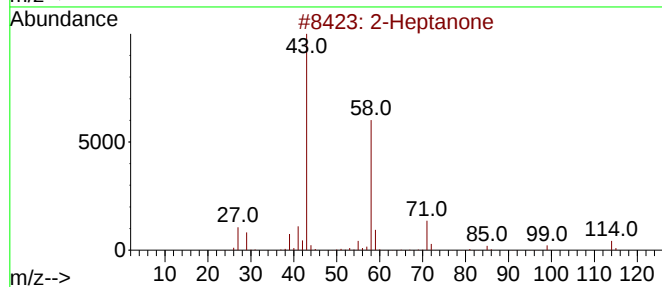
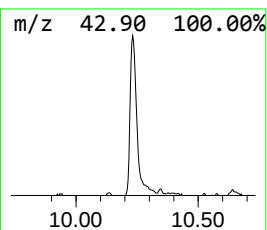
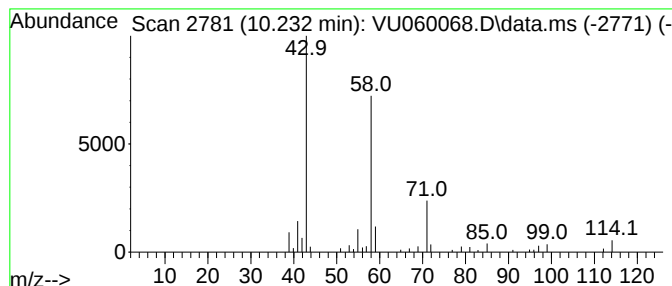
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	0.85 ug/L	59967	Chlorobenzene-d5	9.412

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	91
3	2-Heptanone			114	C7H14O	000110-43-0	90
4	2-Heptanone			114	C7H14O	000110-43-0	90
5	2-Heptanone			114	C7H14O	000110-43-0	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.686	4.5	ug/L	247143	1	6.242	277502	5.0
Propanal, 2,2-d...	4.435	2.1	ug/L	117979	1	6.242	277502	5.0
Hexanal	8.782	0.5	ug/L	36331	2	9.412	352907	5.0
2-Heptanone	10.232	0.8	ug/L	59967	2	9.412	352907	5.0