LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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: VU059518.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	11	20	27	rBV4	3502	5595	1.18%	0.126%
2	1.596	85	95	111	rBV	55058	72873	15.43%	1.636%
3	1.682	111	122	143	rBV	118005	162553	34.41%	3.650%
4	1.908	184	192	211	rVB	49450	68276	14.45%	1.533%
5	2.329	314	323	333	rVB2	4761	7602	1.61%	0.171%
6	2.560	374	395	406	rBV	91310	151652	32.11%	3.405%
7	2.625	406	415	445	rVB	84593	172628	36.55%	3.876%
8	3.194	579	592	611	rVB3	6032	16430	3.48%	0.369%
9	4.435	960	978	996	rBV6	16395	51398	10.88%	1.154%
10	4.618	1023	1035	1054	rBV	66223	172936	36.61%	3.883%
11	5.052	1156	1170	1193	rBV	89797	200784	42.51%	4.508%
12	5.718	1356	1377	1405	rBV2	177187	460165	97.42%	10.333%
13	6.242	1527	1540	1567	rBV	151254	301424	63.81%	6.768%
14	6.682	1664	1677	1695	rBV	106915	214805	45.48%	4.823%
15	6.776	1700	1706	1725	rVB3	4111	9205	1.95%	0.207%
16	6.882	1731	1739	1750	rBV4	5149	10970	2.32%	0.246%
17	7.120	1800	1813	1819	rBV4	4226	8010	1.70%	0.180%
18	7.563	1939	1951	1976	rBV2	44212	82106	17.38%	1.844%
19	7.891	2040	2053	2070	rBV	204321	357527	75.69%	8.028%
20	8.174	2131	2141	2155	rBV2	29026	50409	10.67%	1.132%
21	8.628	2270	2282	2316	rBV	227303	472345	100.00%	10.606%
22	8.785	2322	2331	2348	rVB3	16895	30840	6.53%	0.692%
23	9.412	2514	2526	2545	rBV	233189	393235	83.25%	8.830%
24	9.647	2589	2599	2610	rBV2	6635	11522	2.44%	0.259%
25	10.129	2742	2749	2760	rVB3	4524	6394	1.35%	0.144%
26	10.232	2772	2781	2797	rBV2	34376	58891	12.47%	1.322%
27	10.344	2808	2816	2831	rVB5	4199	7812	1.65%	0.175%
28	10.750	2930	2942	2956	rBV	96241	152552	32.30%	3.425%
29	10.862	2966	2977	2983	rBV3	9196	15428	3.27%	0.346%
30	11.573	3189	3198	3205	rBV6	3374	5462	1.16%	0.123%
31	11.692	3226	3235	3242	rBV5	3223	5079	1.08%	0.114%
32	11.807	3259	3271	3292	rBV	219495	361609	76.56%	8.120%
33	12.065	3343	3351	3357	rBV5	4217	7615	1.61%	0.171%
34	12.187	3378	3389	3413	rBV	200878	336521	71.24%	7.556%
35	12.888	3599	3607	3619	rBV6	6573	10842	2.30%	0.243%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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

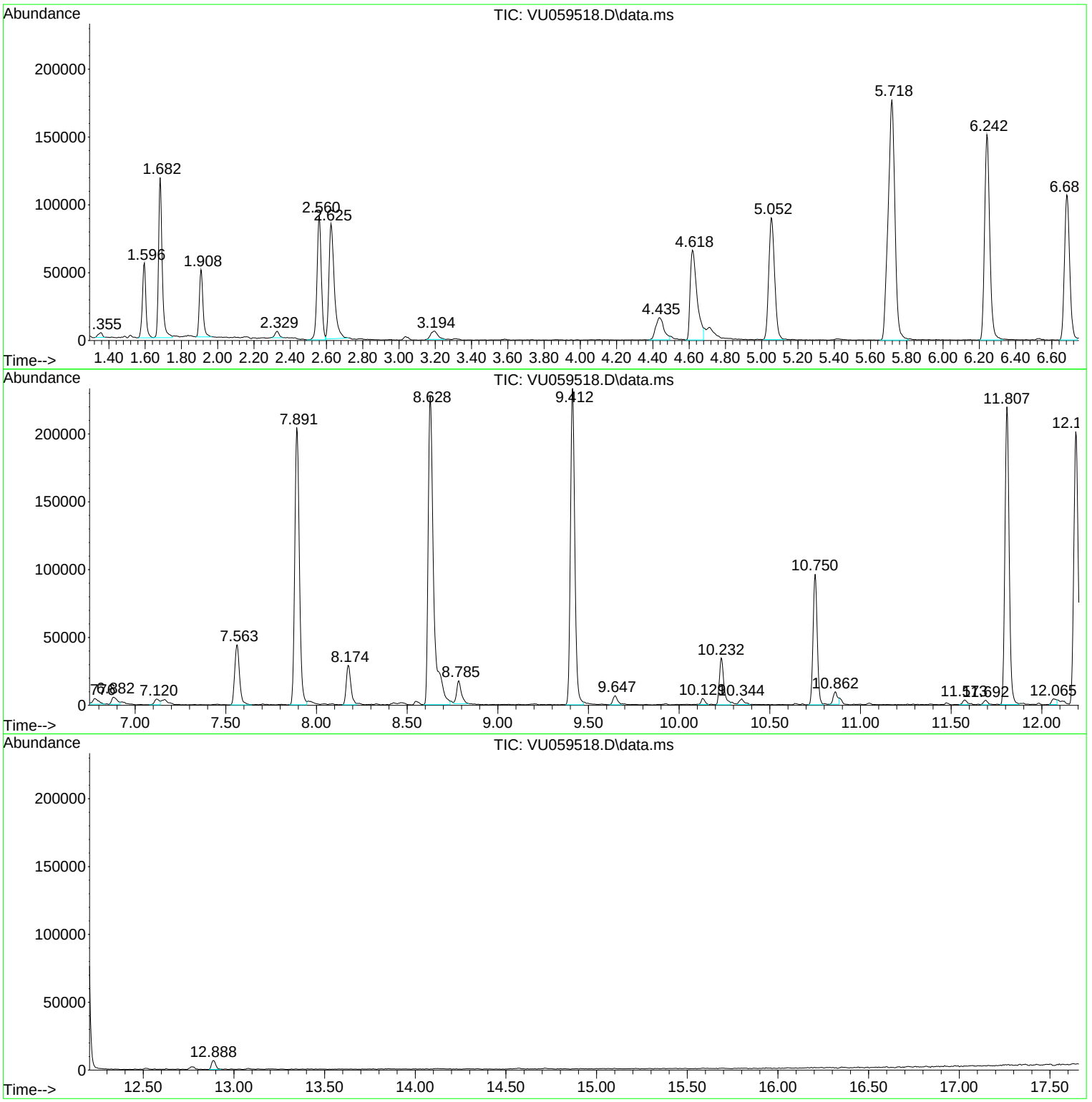
Sum of corrected areas: 4453495

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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

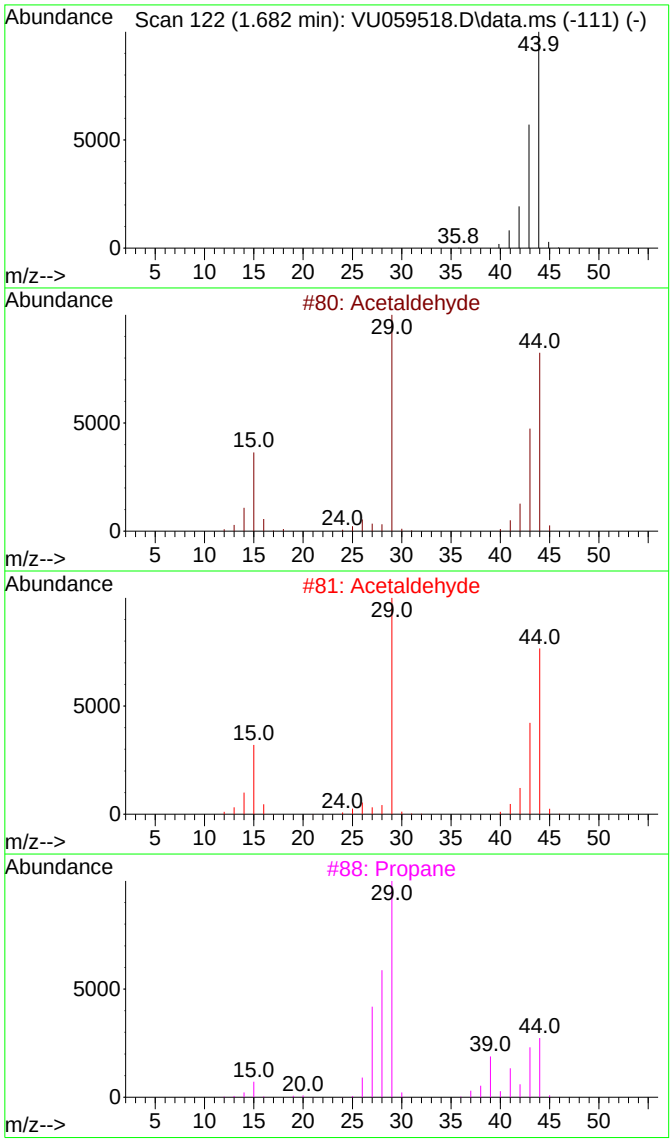
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

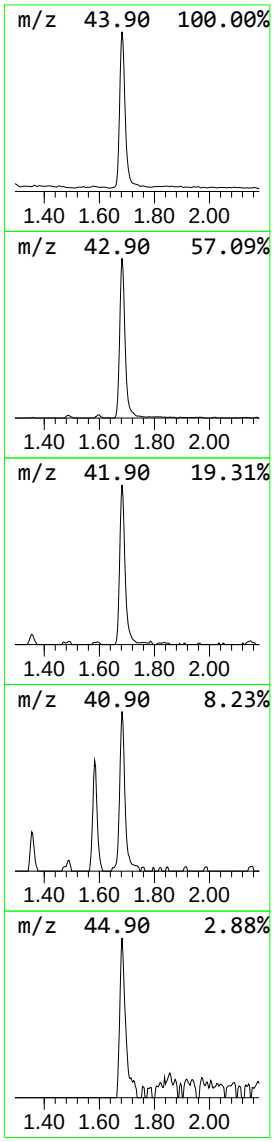
****

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.682	2.70 ug/L	162553	1,4-Difluorobenzene	6.242

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	Propane	44	C3H8	000074-98-6	5
4	Ethylene oxide	44	C2H4O	000075-21-8	5
5	Ethylene oxide	44	C2H4O	000075-21-8	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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

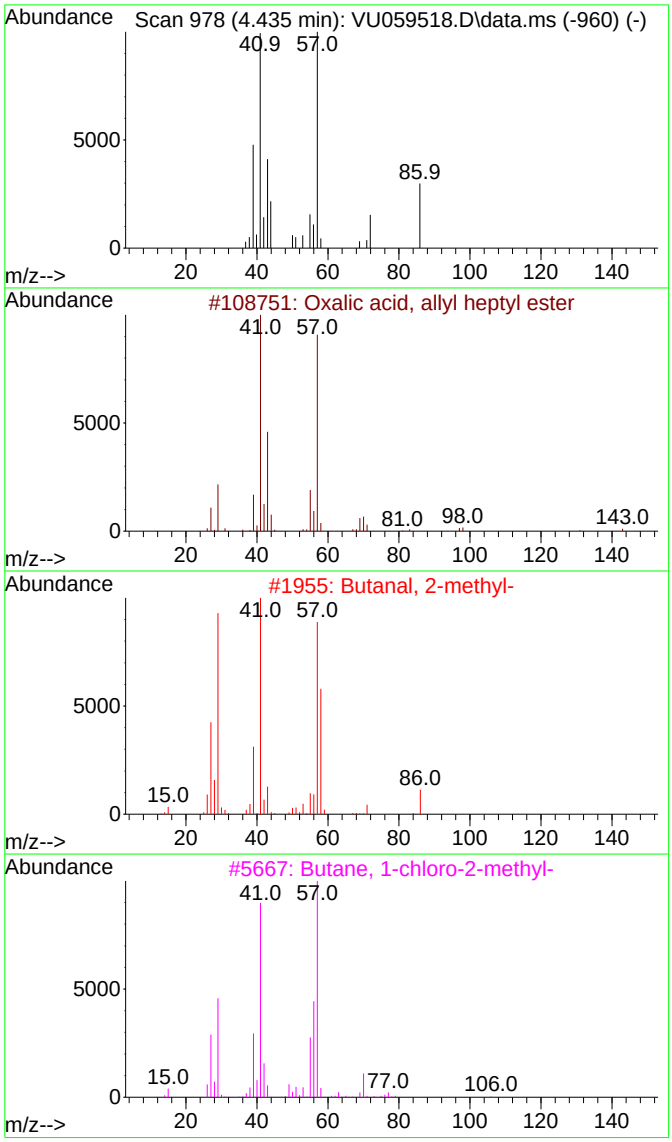
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

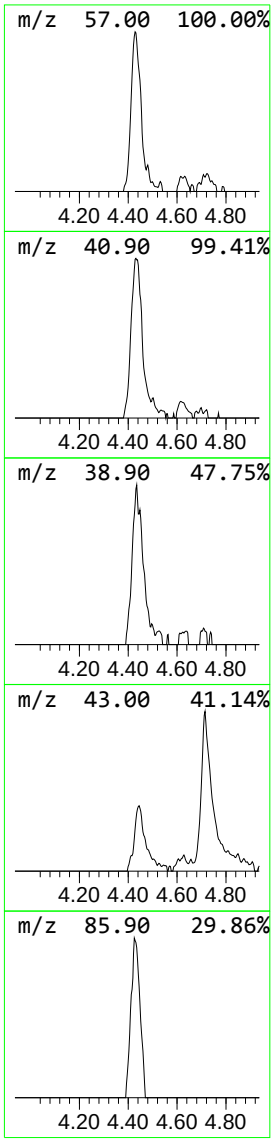
****

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.435	0.85 ug/L	51398	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl heptyl ester	228	C12H20O4	1000309-23-5	35
2	Butanal, 2-methyl-	86	C5H10O	000096-17-3	16
3	Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	12
4	2-Penten-1-ol, (E)-	86	C5H10O	001576-96-1	12
5	1-Hexene	84	C6H12	000592-41-6	12





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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

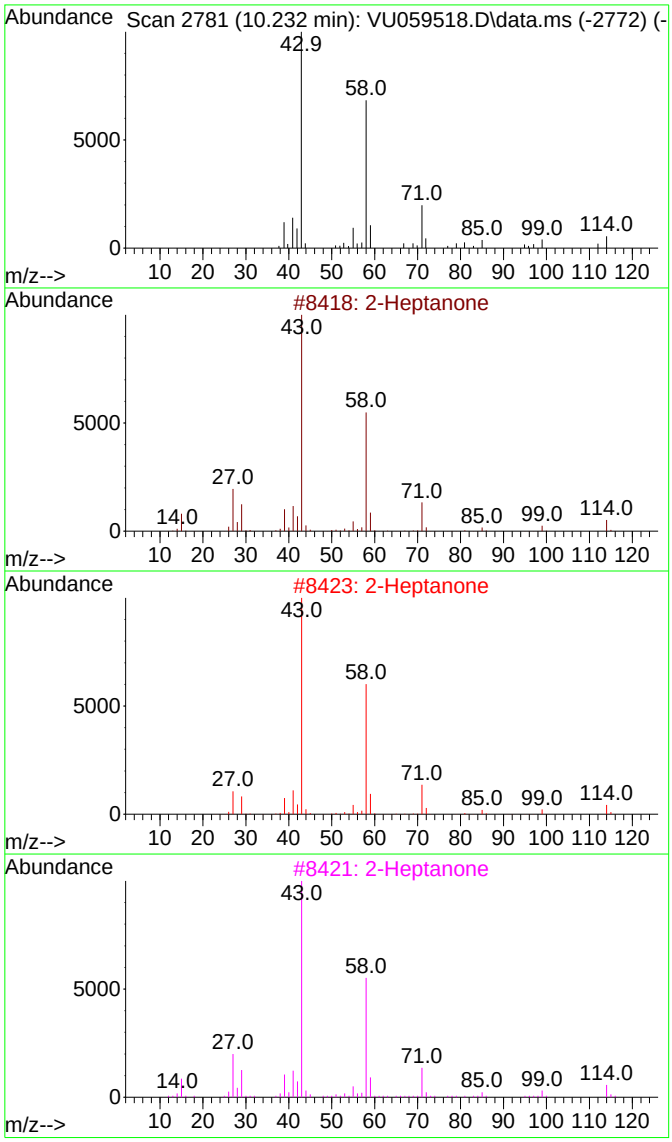
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

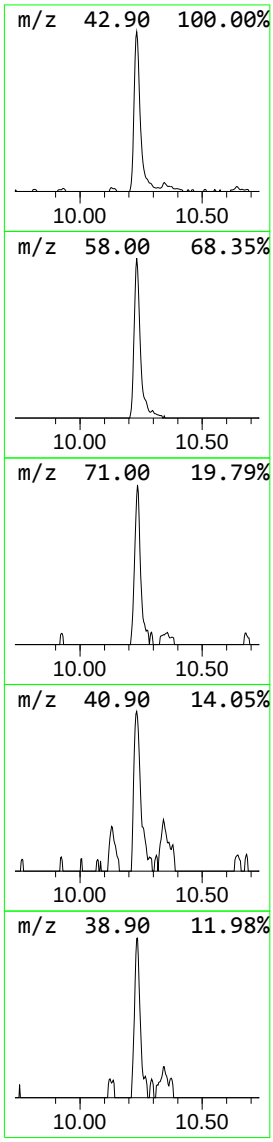
****

Peak Number 4 2-Heptanone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.232	0.75 ug/L	58891	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	90
3	2-Heptanone	114	C7H14O	000110-43-0	90
4	2-Heptanone	114	C7H14O	000110-43-0	86
5	2-Hexanone, 5-methyl-	114	C7H14O	000110-12-3	78





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU062524\
Data File : VU059518.D
Acq On : 26 Jun 2024 11:36
Operator : MD/SY
Sample : P2987-09
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 68 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0T96

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Acetaldehyde	1.682	2.7	ug/L	162553	1	6.242	301424	5.0
unknown-01	4.435	0.8	ug/L	51398	1	6.242	301424	5.0
2-Heptanone	10.232	0.8	ug/L	58891	2	9.412	393235	5.0