LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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\SFAMUTR102423WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU056064.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.361	15	22	38	rVB2	97066	145124	10.84%	1.031%
2	1.489	56	62	67	rVB2	16410	15195	1.14%	0.108%
3	1.599	85	96	112	rVB	198993	259078	19.36%	1.840%
4	1.689	117	124	134	rBV	43449	62490	4.67%	0.444%
5	1.914	185	194	211	rBV	131475	184254	13.77%	1.309%
6	1.994	214	219	229	rVB4	10190	13501	1.01%	0.096%
7	2.567	381	397	410	rBV	285915	489689	36.59%	3.478%
8	2.647	410	422	440	rVV	26705	74922	5.60%	0.532%
9	2.792	456	467	483	rBV	55576	94585	7.07%	0.672%
10	3.181	576	588	612	rVB2	26867	64924	4.85%	0.461%
11	3.586	697	714	732	rBV3	12322	32355	2.42%	0.230%
12	4.447	964	982	1006	rBV6	35163	110761	8.28%	0.787%
13	4.631	1024	1039	1085	rBV	145401	521025	38.93%	3.701%
14	5.058	1156	1172	1199	rBV	256616	603465	45.09%	4.287%
15	5.721	1358	1378	1407	rBV2	507527	1334796	99.73%	9.481%
16	6.245	1527	1541	1572	rBV	452553	886193	66.21%	6.295%
17	6.685	1661	1678	1701	rBV	303024	605421	45.23%	4.300%
18	6.881	1729	1739	1755	rBV3	24803	49317	3.68%	0.350%
19	7.563	1938	1951	1969	rBV	148420	274370	20.50%	1.949%
20	7.894	2038	2054	2074	rBV	598521	1092716	81.64%	7.762%
21	8.177	2132	2142	2156	rBV	88083	155997	11.65%	1.108%
22	8.264	2162	2169	2187	rVB8	11647	24844	1.86%	0.176%
23	8.483	2223	2237	2248	rBV4	24428	54624	4.08%	0.388%
24	8.560	2252	2261	2272	rVB7	8383	16424	1.23%	0.117%
25	8.634	2272	2284	2321	rBV2	598413	1338460	100.00%	9.507%
26	8.785	2321	2331	2354	rVB2	76395	148666	11.11%	1.056%
27	9.415	2514	2527	2550	rBV	624462	1095012	81.81%	7.778%
28	10.341	2806	2815	2839	rVB2	76454	133659	9.99%	0.949%
29	10.753	2929	2943	2958	rBV	227032	370905	27.71%	2.635%
30	10.888	2974	2985	2996	rBV	34923	57581	4.30%	0.409%
31	11.042	3022	3033	3047	rBV5	24292	51512	3.85%	0.366%
32	11.122	3047	3058	3061	rBV5	12226	20225	1.51%	0.144%
33	11.630	3207	3216	3222	rVV2	10398	14723	1.10%	0.105%
34	11.682	3222	3232	3245	rVV	265266	438792	32.78%	3.117%
35	11.746	3246	3252	3260	rVV	25754	43029	3.21%	0.306%
36	11.807	3260	3271	3297	rVB	647167	1079613	80.66%	7.669%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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\SFAMUTR102423WMA.M
Title : TRACE VOA SFAM1.0

37	12.058	3333	3349	3365	rBV	61135	138676	10.36%	0.985%
38	12.190	3378	3390	3412	rVB	570358	951625	71.10%	6.760%
39	12.335	3424	3435	3442	rBV7	13860	24188	1.81%	0.172%
40	12.772	3560	3571	3584	rBV2	13177	22978	1.72%	0.163%
41	12.881	3592	3605	3632	rBV	606943	968721	72.38%	6.881%
42	13.984	3939	3948	3961	rBV7	7967	13740	1.03%	0.098%

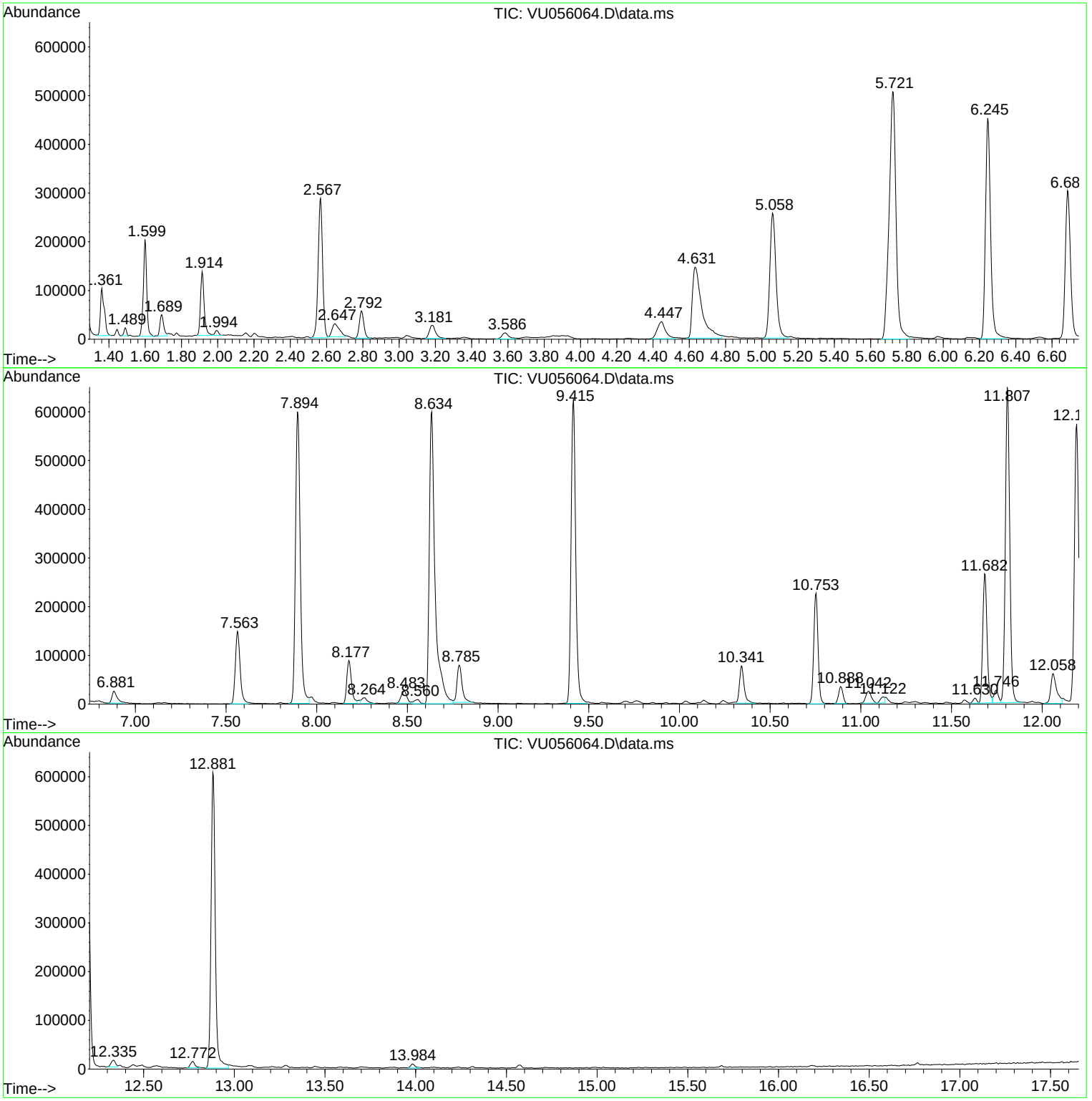
Sum of corrected areas: 14078175

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.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\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

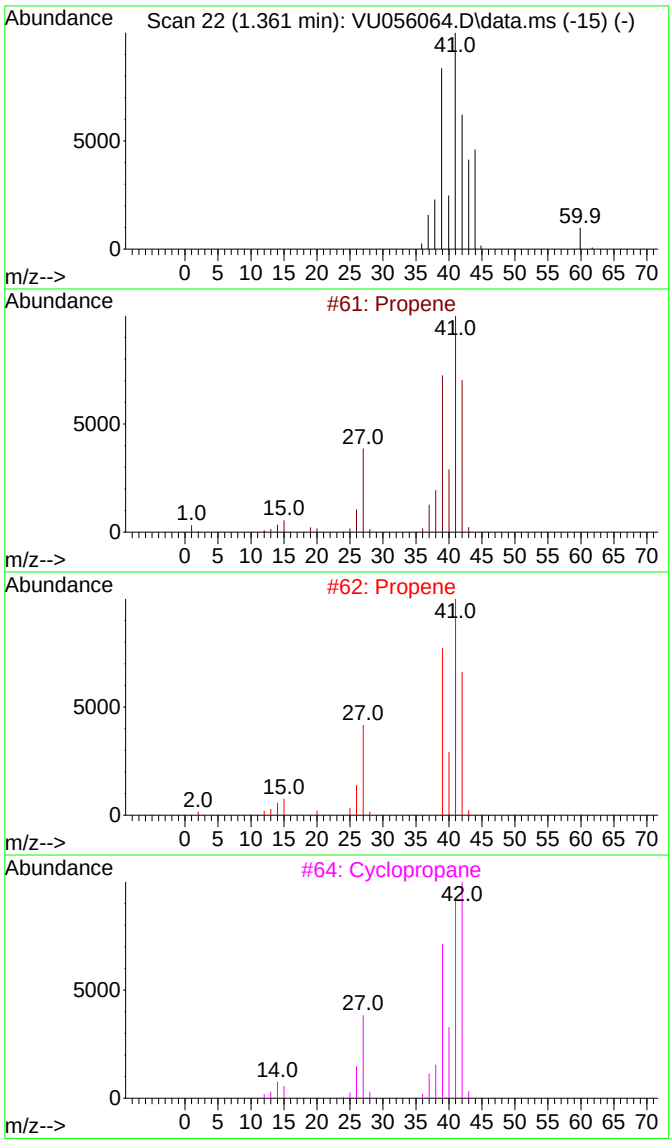
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

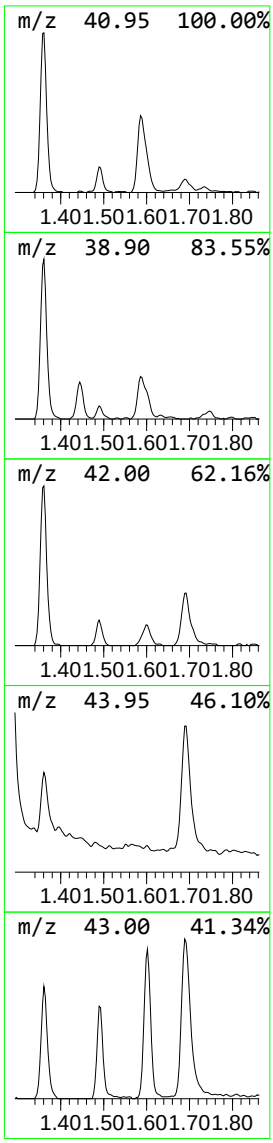
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.361	0.82 ug/L	145124	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Propene	42	C3H6	000115-07-1	40
3	Cyclopropane	42	C3H6	000075-19-4	7
4	Cyclopropane	42	C3H6	000075-19-4	7
5	Cyclopropene	40	C3H4	002781-85-3	5





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

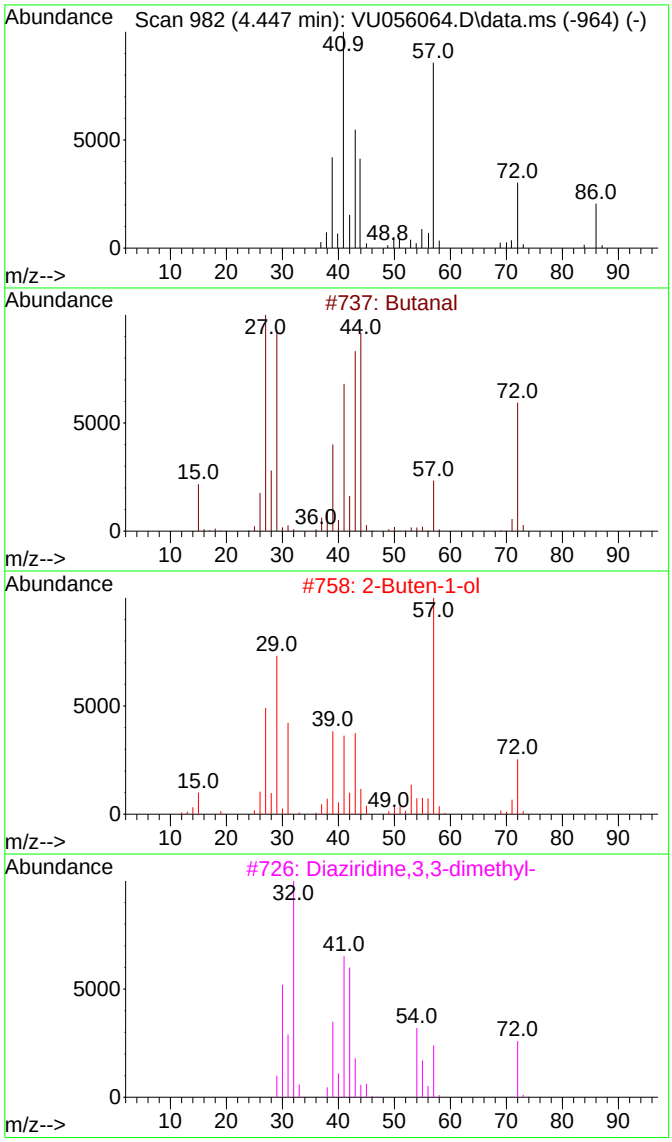
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

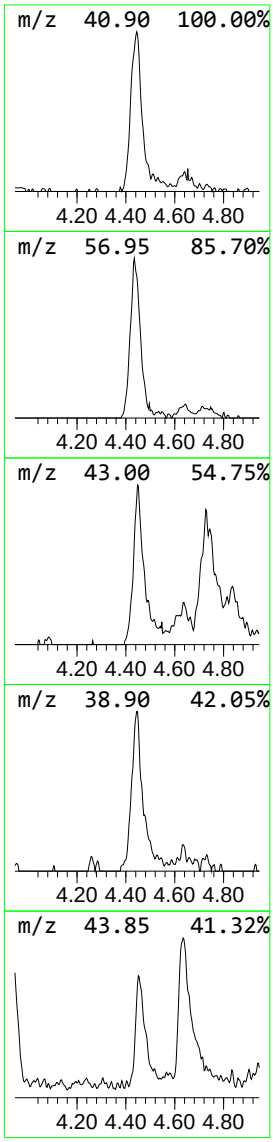
****

Peak Number 2 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.447	0.62 ug/L	110761	1,4-Difluorobenzene	6.245

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	43
2	2-Buten-1-ol	72	C4H8O	006117-91-5	43
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38
4	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	35
5	2-Propen-1-ol, 2-methyl-	72	C4H8O	000513-42-8	32





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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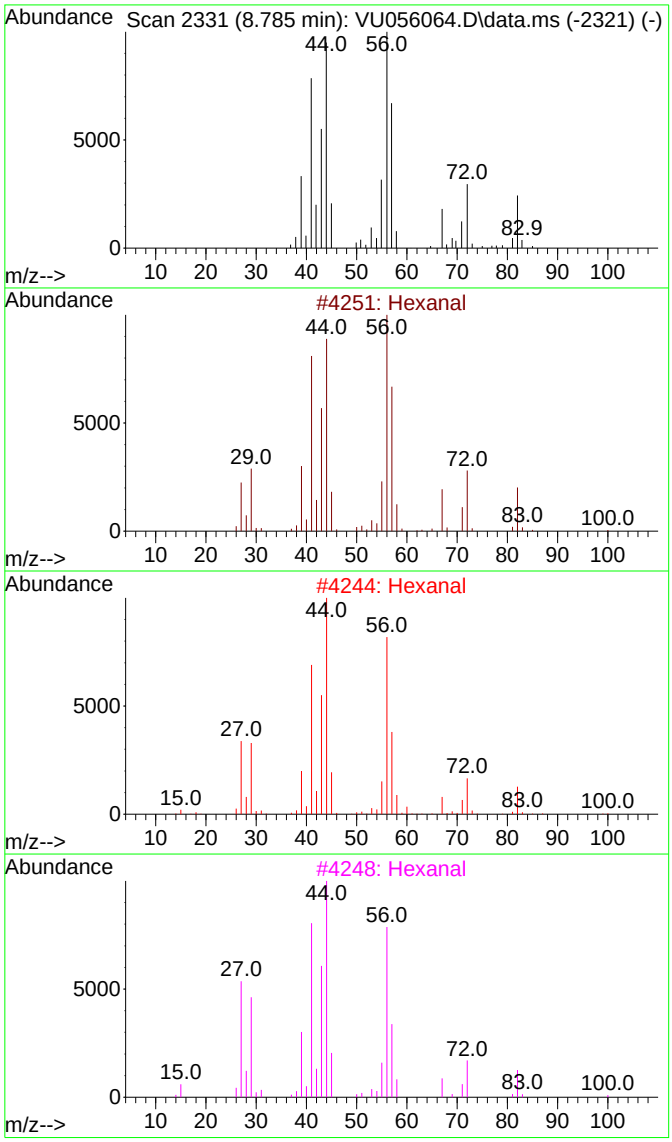
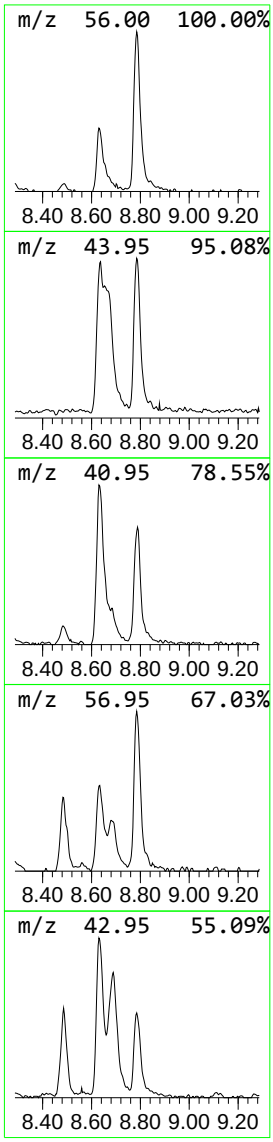
Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	0.68 ug/L	148666	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	78
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	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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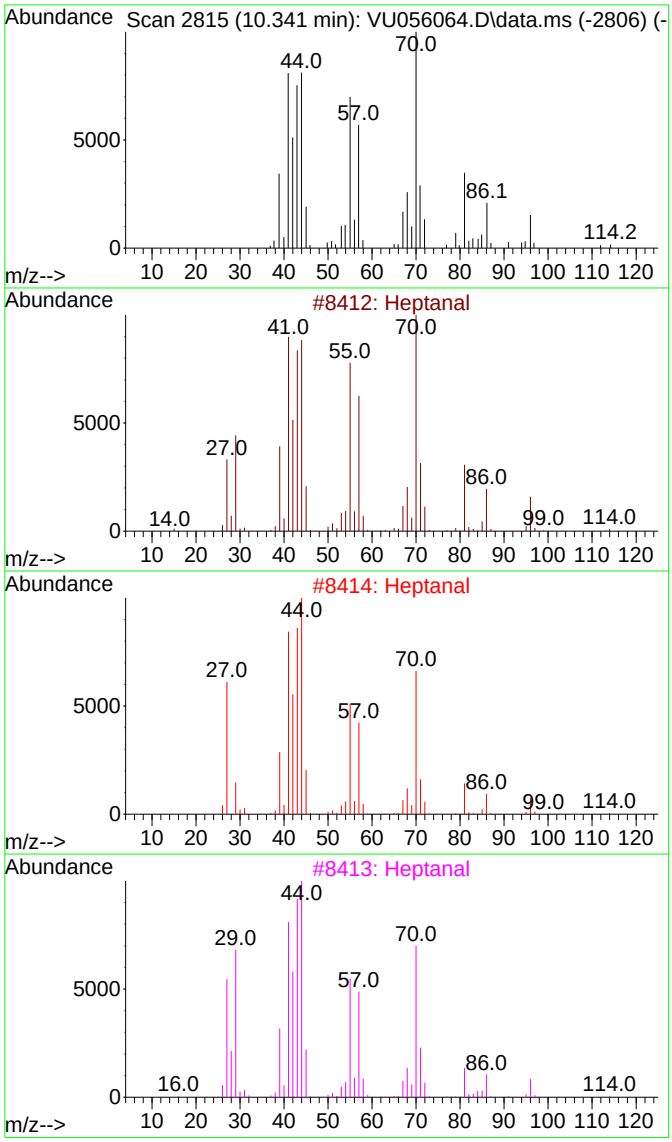
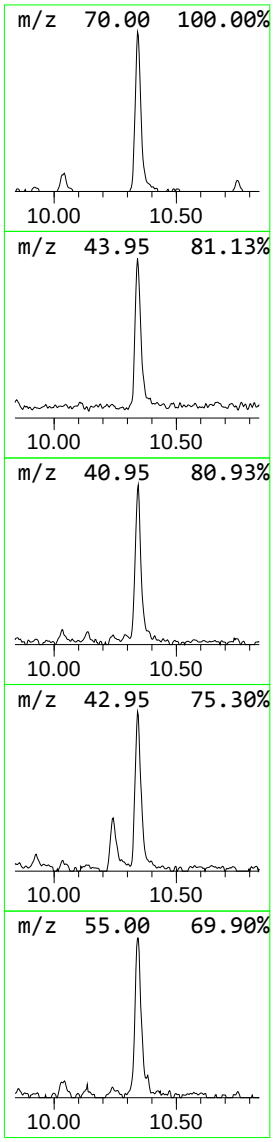
Peak Number 5 Heptanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.341	0.61 ug/L	133659	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	96
2	Heptanal	114	C7H14O	000111-71-7	95
3	Heptanal	114	C7H14O	000111-71-7	83
4	Heptanal	114	C7H14O	000111-71-7	83
5	Heptanal	114	C7H14O	000111-71-7	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

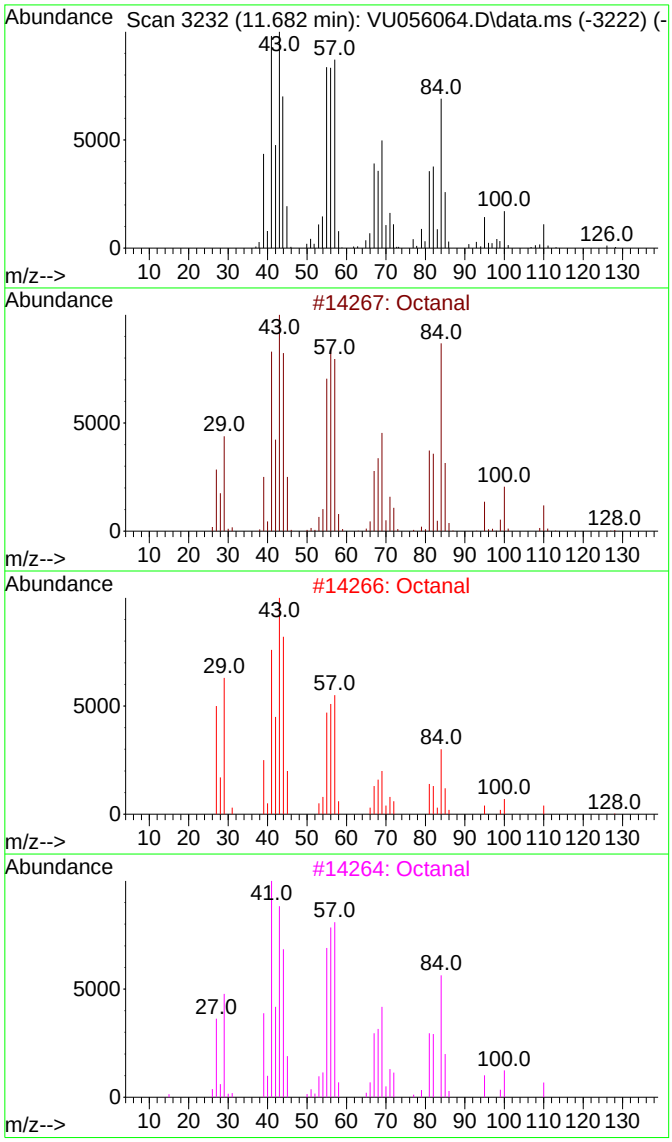
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

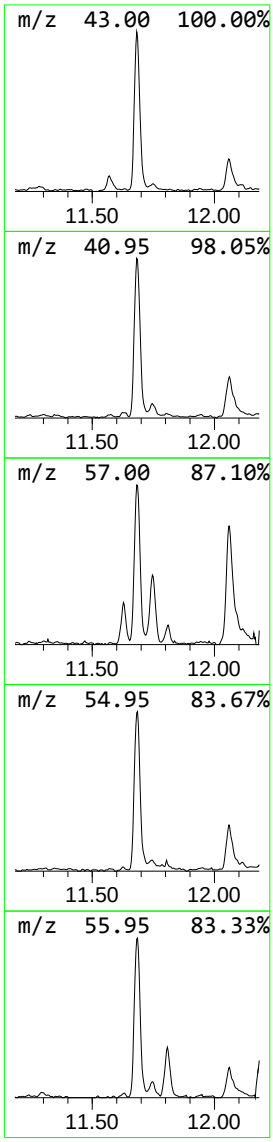
****

Peak Number 6 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.682	2.03 ug/L	438792	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	98
2	Octanal	128	C8H16O	000124-13-0	94
3	Octanal	128	C8H16O	000124-13-0	91
4	Octanal	128	C8H16O	000124-13-0	87
5	Octanal	128	C8H16O	000124-13-0	81





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Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

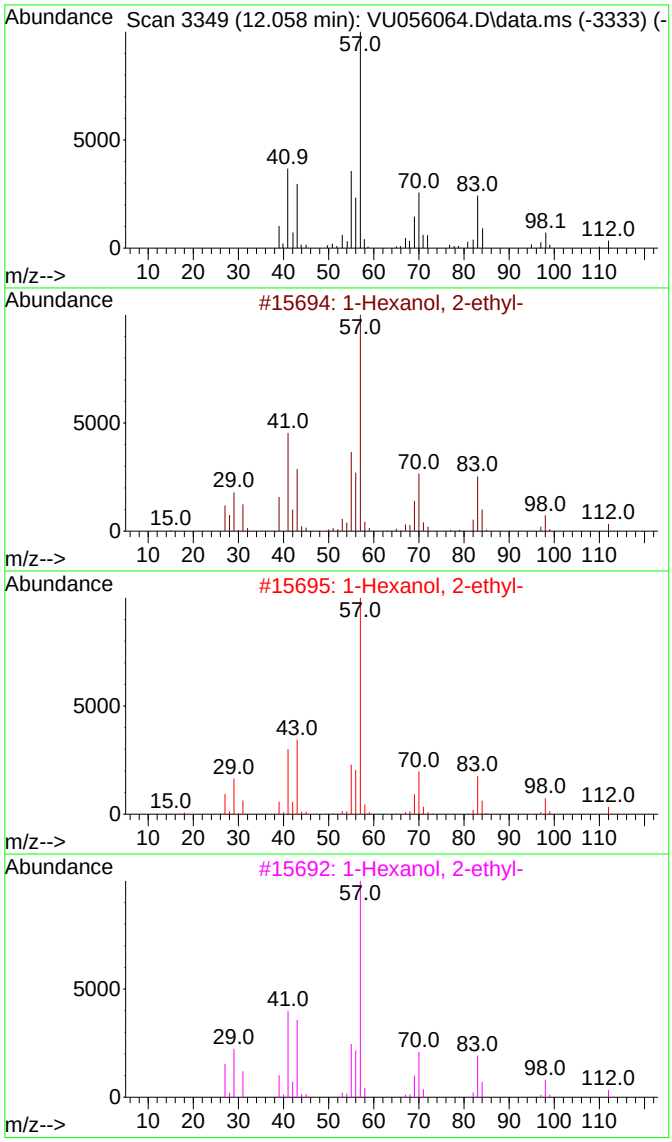
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

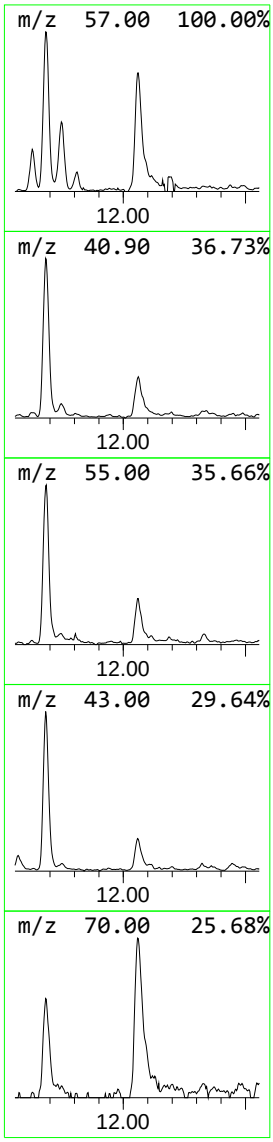
****

Peak Number 7 1-Hexanol, 2-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.058	0.64 ug/L	138676	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72





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Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

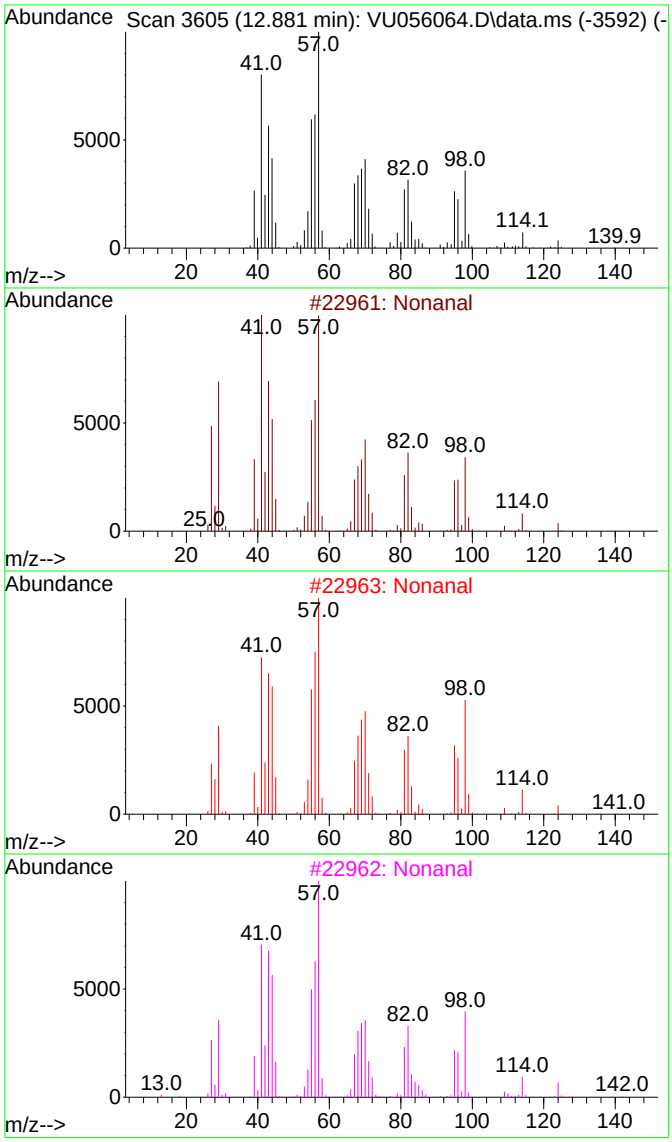
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

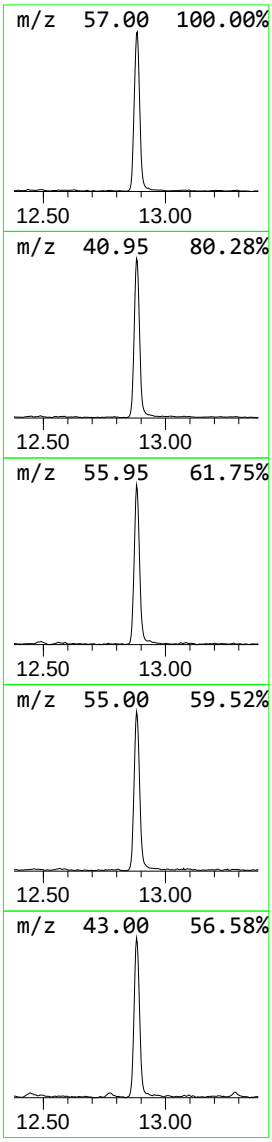
****

Peak Number 8 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.881	4.49 ug/L	968721	1,4-Dichlorobenzene-d4	11.810

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanal	142	C9H18O	000124-19-6	91
2	Nonanal	142	C9H18O	000124-19-6	90
3	Nonanal	142	C9H18O	000124-19-6	72
4	Cyclohexanol, 2-methyl-, trans-	114	C7H14O	007443-52-9	38
5	Cyclohexanol, 2-methyl-	114	C7H14O	000583-59-5	38





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110223\
Data File : VU056064.D
Acq On : 02 Nov 2023 14:32
Operator : MD/SY
Sample : 05052-04
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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.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
(DEL) Alkane: S...	1.361	0.8	ug/L	145124	1	6.245	886193	5.0
unknown-01	4.447	0.6	ug/L	110761	1	6.245	886193	5.0
Hexanal	8.785	0.7	ug/L	148666	2	9.415	1095010	5.0
Heptanal	10.341	0.6	ug/L	133659	2	9.415	1095010	5.0
Octanal	11.682	2.0	ug/L	438792	3	11.810	1079610	5.0
1-Hexanol, 2-et...	12.058	0.6	ug/L	138676	3	11.810	1079610	5.0
Nonanal	12.881	4.5	ug/L	968721	3	11.810	1079610	5.0