LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 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: VU056050.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	40	rVB2	111783	171719	12.76%	1.251%
2	1.441	42	47	54	rVB2	12490	14016	1.04%	0.102%
3	1.490	57	62	67	rBV	15729	14294	1.06%	0.104%
4	1.599	85	96	106	rBV2	135755	191356	14.22%	1.394%
5	1.689	116	124	135	rBV	54247	80761	6.00%	0.588%
6	1.914	185	194	210	rVV	98141	138320	10.28%	1.008%
7	1.994	213	219	228	rVB4	10531	14500	1.08%	0.106%
8	2.563	381	396	410	rBV2	191818	339232	25.20%	2.472%
9	2.641	410	420	455	rVB	41429	126863	9.42%	0.924%
10	2.792	456	467	479	rBV	69049	117535	8.73%	0.856%
11	3.043	533	545	554	rBV3	7054	13854	1.03%	0.101%
12	3.184	574	589	605	rBV	19257	48891	3.63%	0.356%
13	3.579	697	712	730	rBV3	15002	39775	2.95%	0.290%
14	4.444	962	981	1005	rBV6	44955	142464	10.58%	1.038%
15	4.631	1026	1039	1086	rBV2	157718	531491	39.48%	3.873%
16	4.814	1089	1096	1113	rVB3	14957	35505	2.64%	0.259%
17	5.058	1154	1172	1203	rBV	225461	525502	39.04%	3.829%
18	5.721	1354	1378	1409	rBV2	420239	1125491	83.61%	8.201%
19	6.245	1528	1541	1573	rBV	448364	897147	66.65%	6.537%
20	6.685	1665	1678	1702	rBV2	271438	527545	39.19%	3.844%
21	6.882	1730	1739	1759	rBV2	30240	62525	4.64%	0.456%
22	7.563	1936	1951	1975	rBV	120619	224218	16.66%	1.634%
23	7.894	2034	2054	2072	rBV	464644	848012	63.00%	6.179%
24	8.177	2131	2142	2153	rBV2	71244	126576	9.40%	0.922%
25	8.258	2161	2167	2183	rVB5	13943	26495	1.97%	0.193%
26	8.483	2223	2237	2250	rBV3	30401	71303	5.30%	0.520%
27	8.550	2250	2258	2270	rVB6	9380	17367	1.29%	0.127%
28	8.631	2271	2283	2321	rBV2	613805	1346133	100.00%	9.809%
29	8.785	2321	2331	2357	rVB2	96359	182478	13.56%	1.330%
30	9.415	2514	2527	2556	rBV	618698	1093335	81.22%	7.967%
31	9.701	2605	2616	2626	rBV7	6190	13986	1.04%	0.102%
32	10.242	2775	2784	2792	rBV2	8795	15193	1.13%	0.111%
33	10.341	2805	2815	2836	rVB2	90479	159018	11.81%	1.159%
34	10.753	2929	2943	2959	rBV	219263	360524	26.78%	2.627%
35	10.891	2975	2986	3002	rVB	49655	81023	6.02%	0.590%
36	11.042	3012	3033	3047	rBV6	29607	71915	5.34%	0.524%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 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	11.116	3047	3056	3057	rBV3	14732	14876	1.11%	0.108%
38	11.573	3187	3198	3207	rBV3	9583	16415	1.22%	0.120%
39	11.627	3207	3215	3221	rVV2	9269	13691	1.02%	0.100%
40	11.685	3221	3233	3245	rVV2	342392	554663	41.20%	4.042%
41	11.746	3246	3252	3260	rVV2	27354	45402	3.37%	0.331%
42	11.807	3260	3271	3291	rVB	624462	1045057	77.63%	7.615%
43	12.061	3336	3350	3378	rBV3	65799	167785	12.46%	1.223%
44	12.190	3378	3390	3407	rVV	477825	789228	58.63%	5.751%
45	12.332	3424	3434	3444	rBV6	18083	33576	2.49%	0.245%
46	12.769	3554	3570	3579	rBV3	21655	36851	2.74%	0.269%
47	12.881	3594	3605	3626	rBV	774127	1194601	88.74%	8.704%
48	13.984	3939	3948	3960	rBV9	8695	15477	1.15%	0.113%

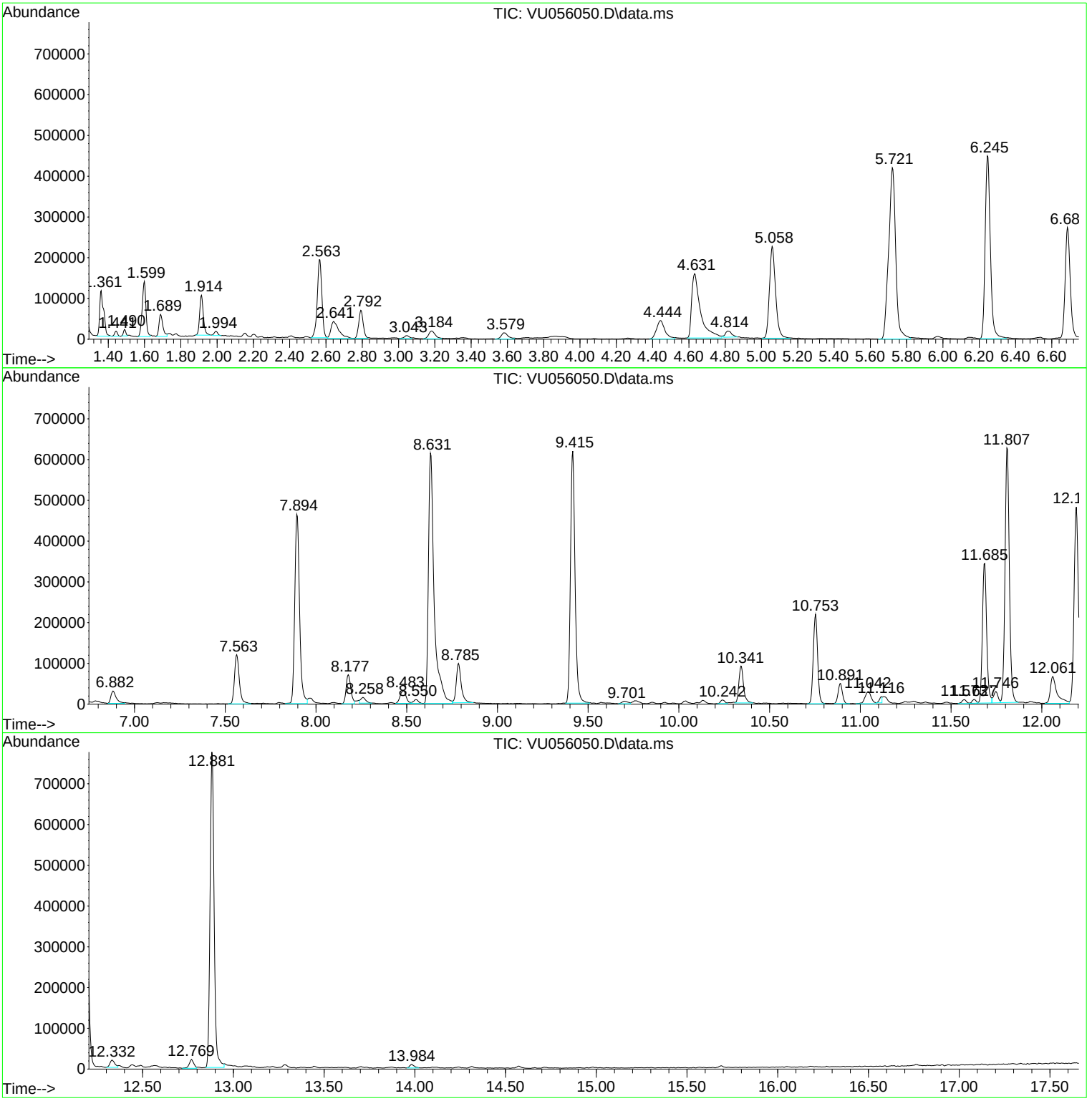
Sum of corrected areas: 13723984

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 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\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

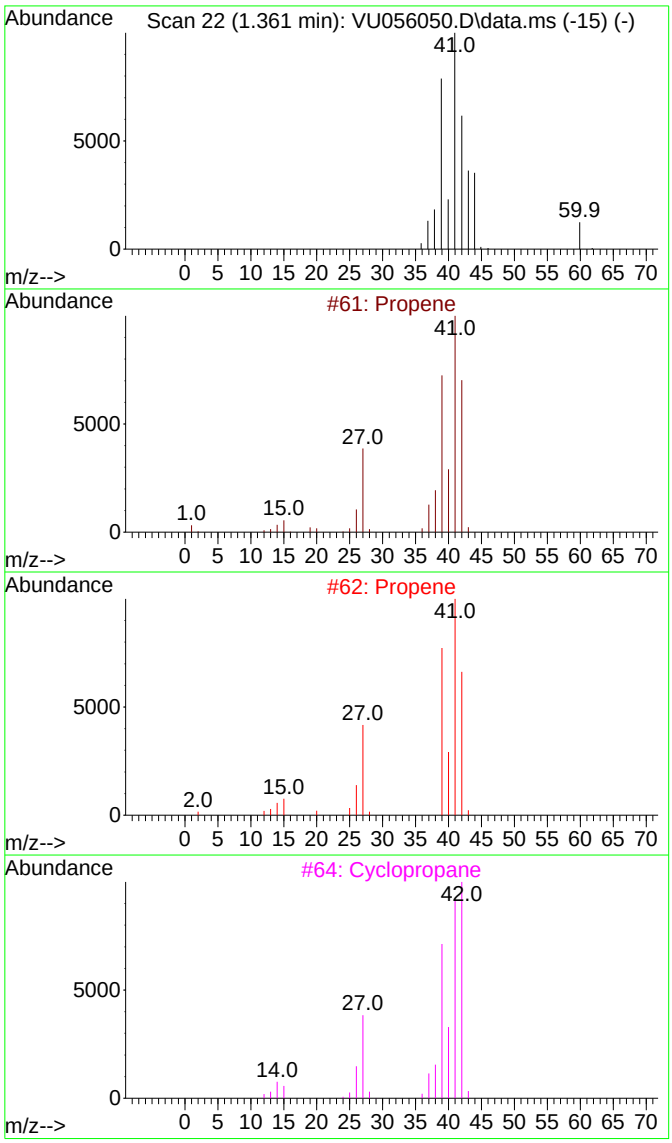
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR102423WMA.M
Quant Title : TRACE VOA SFAM1.0

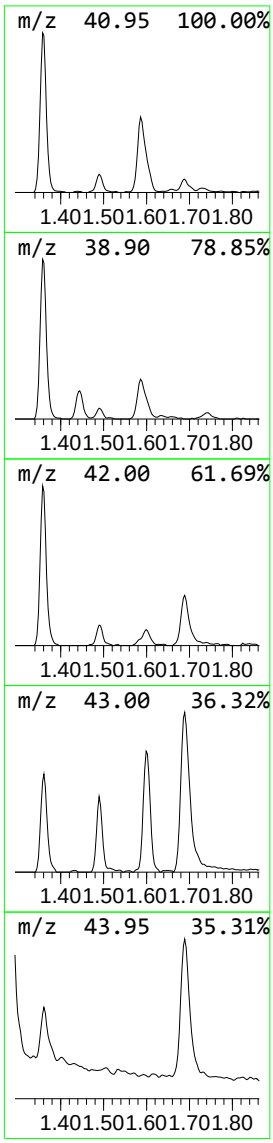
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.361	0.96 ug/L	171719	1,4-Difluorobenzene	6.248

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	86
2	Propene	42	C3H6	000115-07-1	50
3	Cyclopropane	42	C3H6	000075-19-4	10
4	Cyclopropane	42	C3H6	000075-19-4	10
5	Methylenecyclopropane	54	C4H6	006142-73-0	9





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

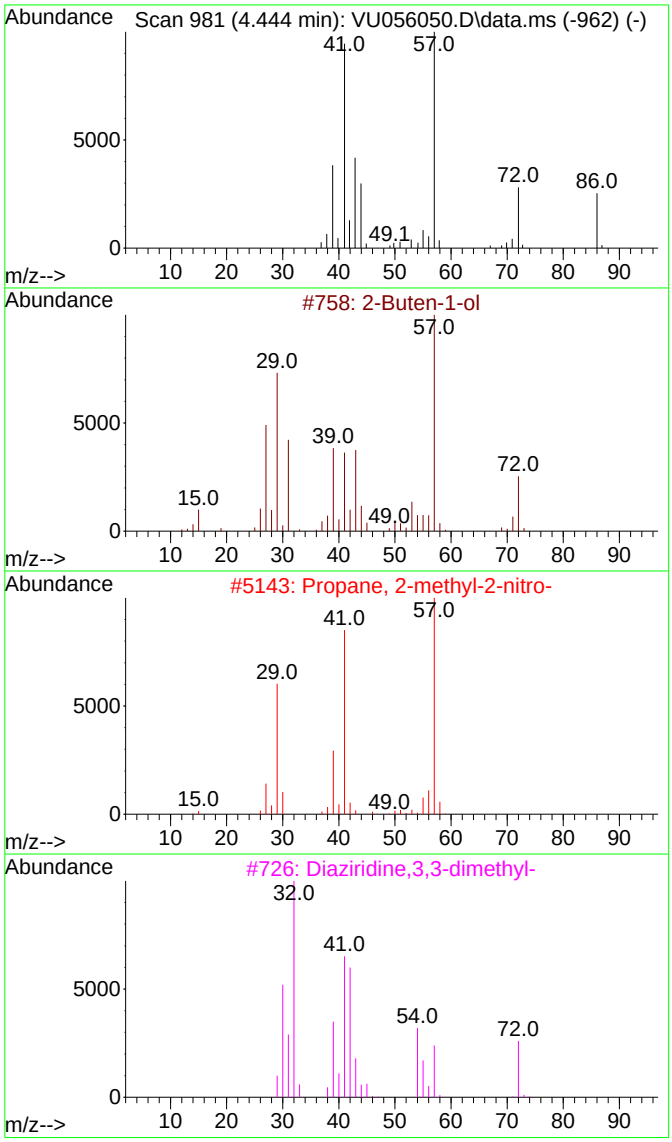
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

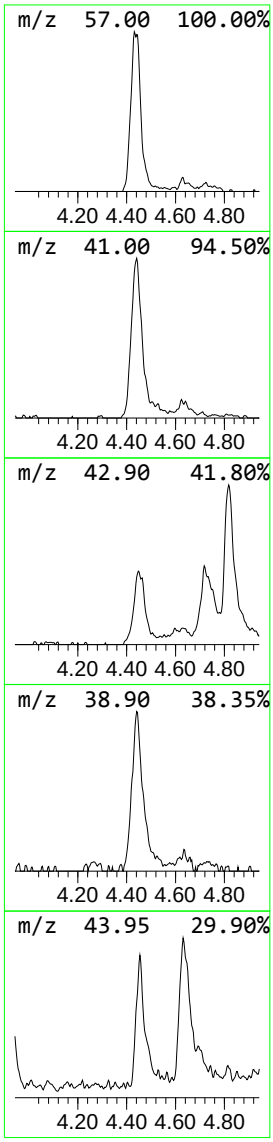
****

Peak Number 2 2-Buten-1-ol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.444	0.79 ug/L	142464	1,4-Difluorobenzene	6.248

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Buten-1-ol	72	C4H8O	006117-91-5	50
2	Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	43
3	Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	43
4	Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	38
5	2-Buten-1-ol, (E)-	72	C4H8O	000504-61-0	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

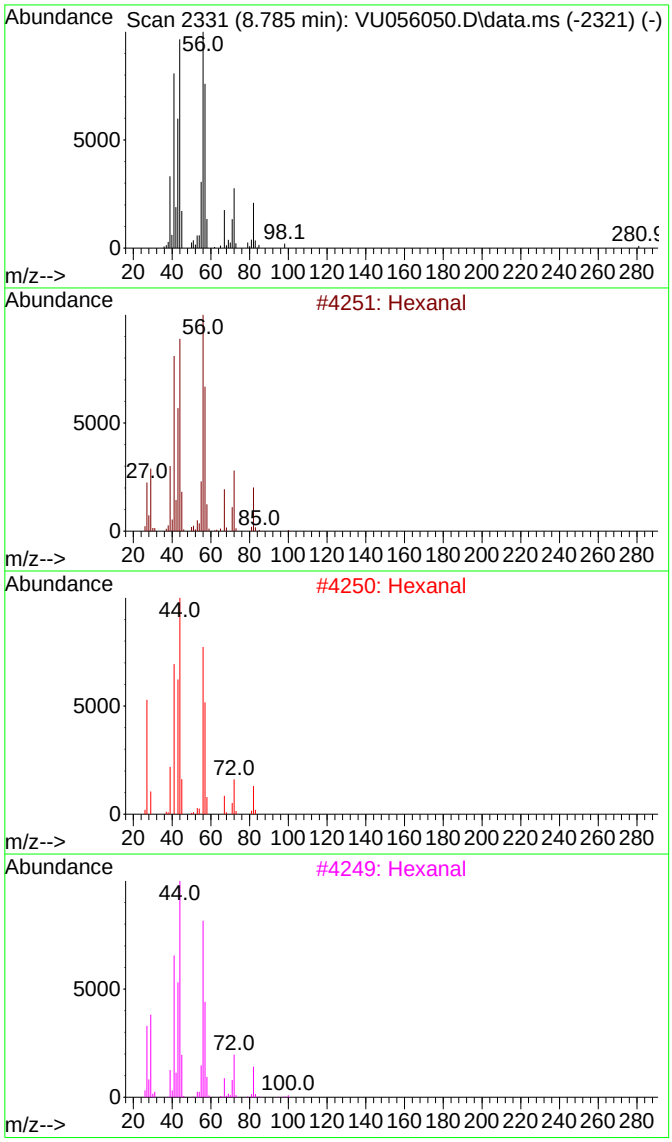
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

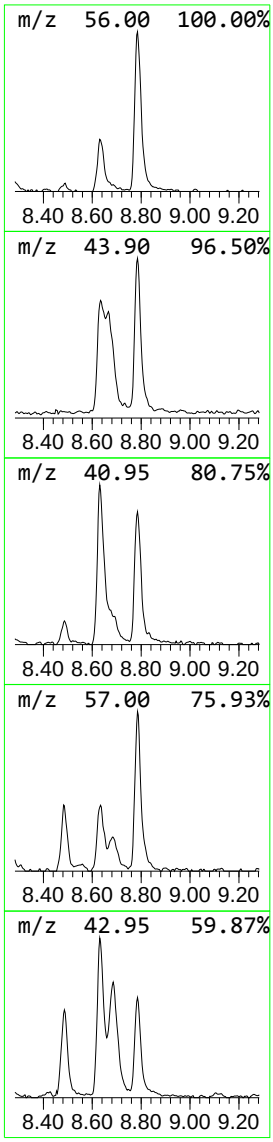
****

Peak Number 4 Hexanal Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.785	0.83 ug/L	182478	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	90
3	Hexanal	100	C6H12O	000066-25-1	90
4	Hexanal	100	C6H12O	000066-25-1	83
5	Hexanal	100	C6H12O	000066-25-1	83





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

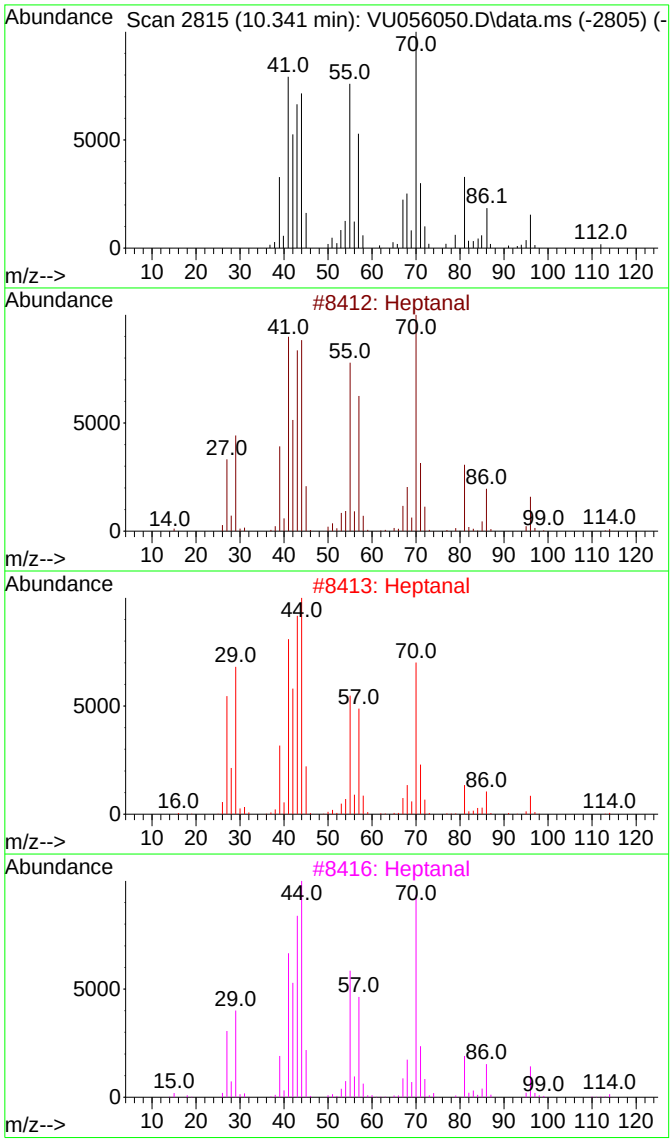
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

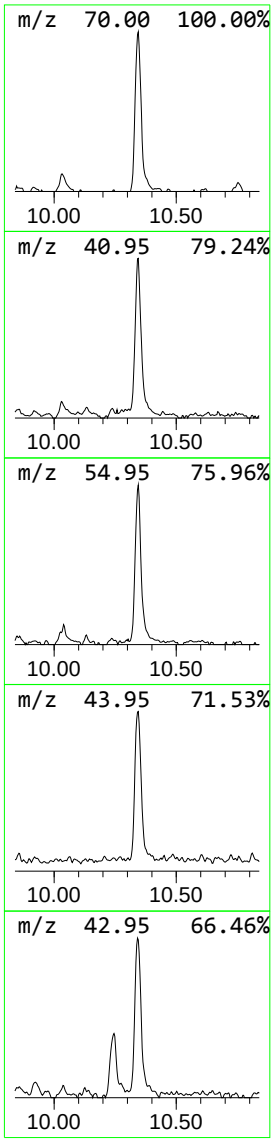
****

Peak Number 5 Heptanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.341	0.73 ug/L	159018	Chlorobenzene-d5	9.415

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptanal	114	C7H14O	000111-71-7	86
2	Heptanal	114	C7H14O	000111-71-7	78
3	Heptanal	114	C7H14O	000111-71-7	72
4	Heptanal	114	C7H14O	000111-71-7	72
5	Heptanal	114	C7H14O	000111-71-7	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

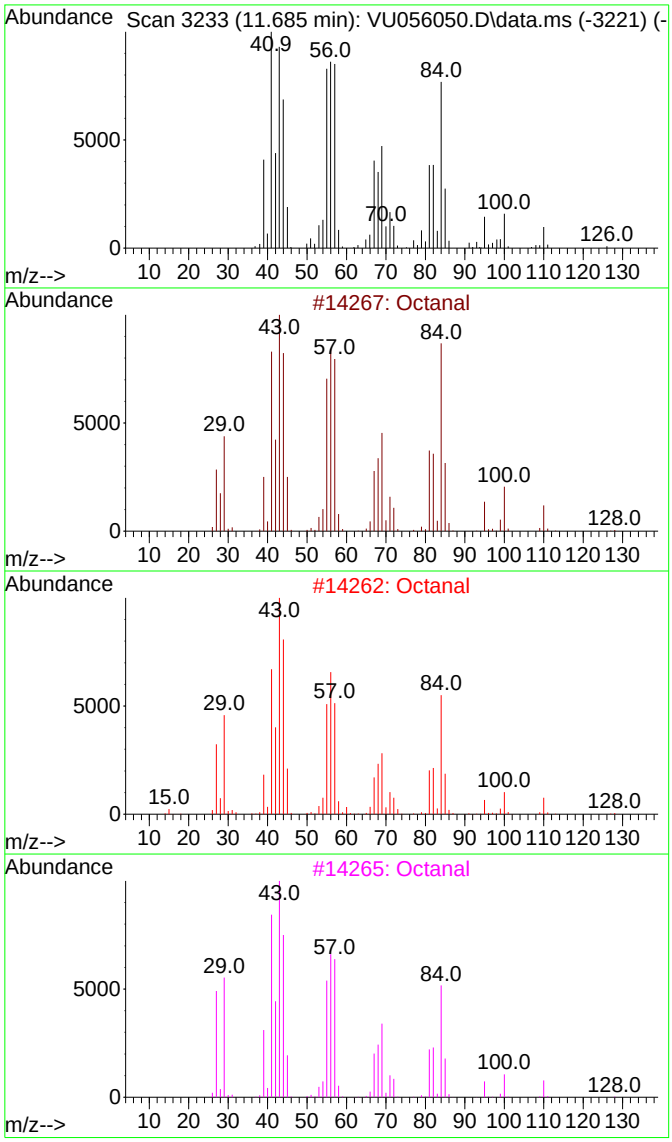
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

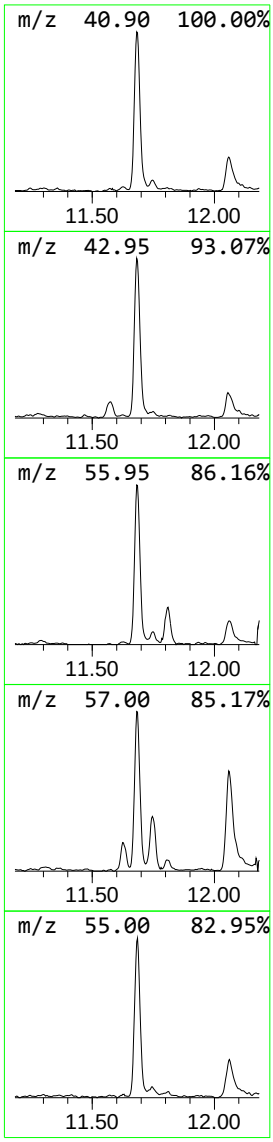
****

Peak Number 6 Octanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.685	2.65 ug/L	554663	1,4-Dichlorobenzene-d4	11.811

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octanal	128	C8H16O	000124-13-0	91
2	Octanal	128	C8H16O	000124-13-0	86
3	Octanal	128	C8H16O	000124-13-0	83
4	Octanal	128	C8H16O	000124-13-0	64
5	Octanal	128	C8H16O	000124-13-0	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

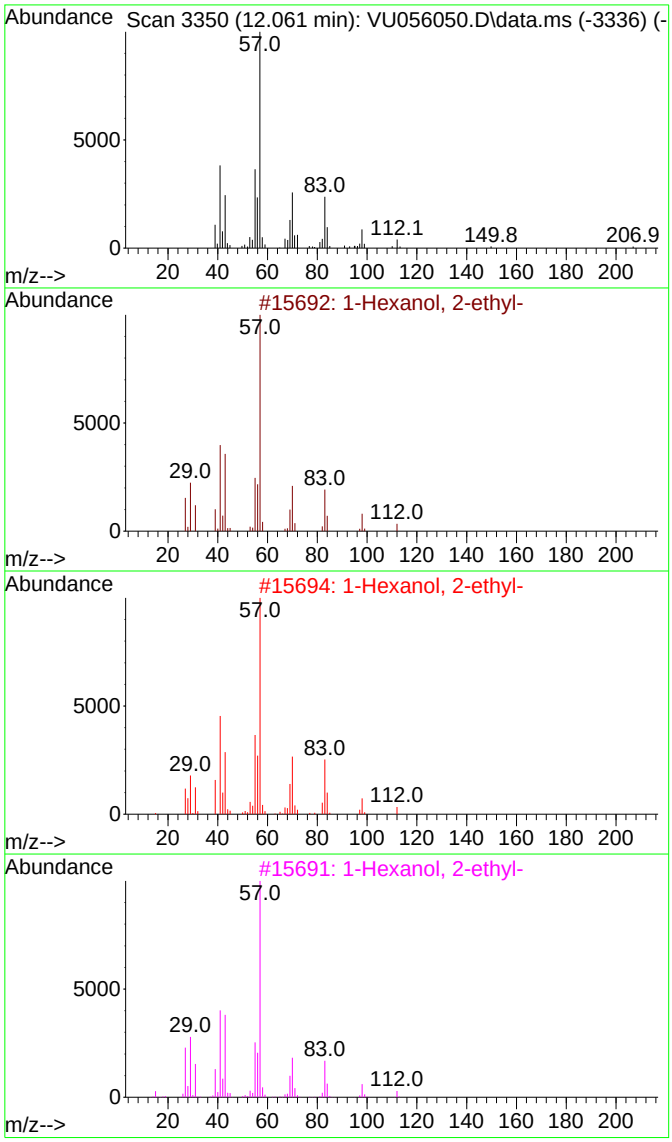
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

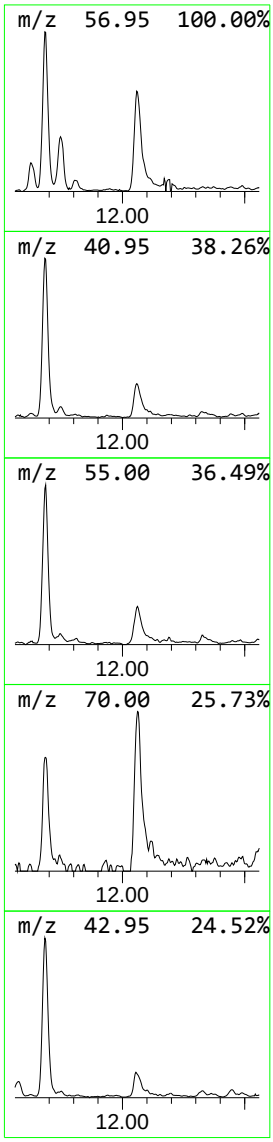
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.061	0.80 ug/L	167785	1,4-Dichlorobenzene-d4	11.811

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	90
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	83
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0AM2

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

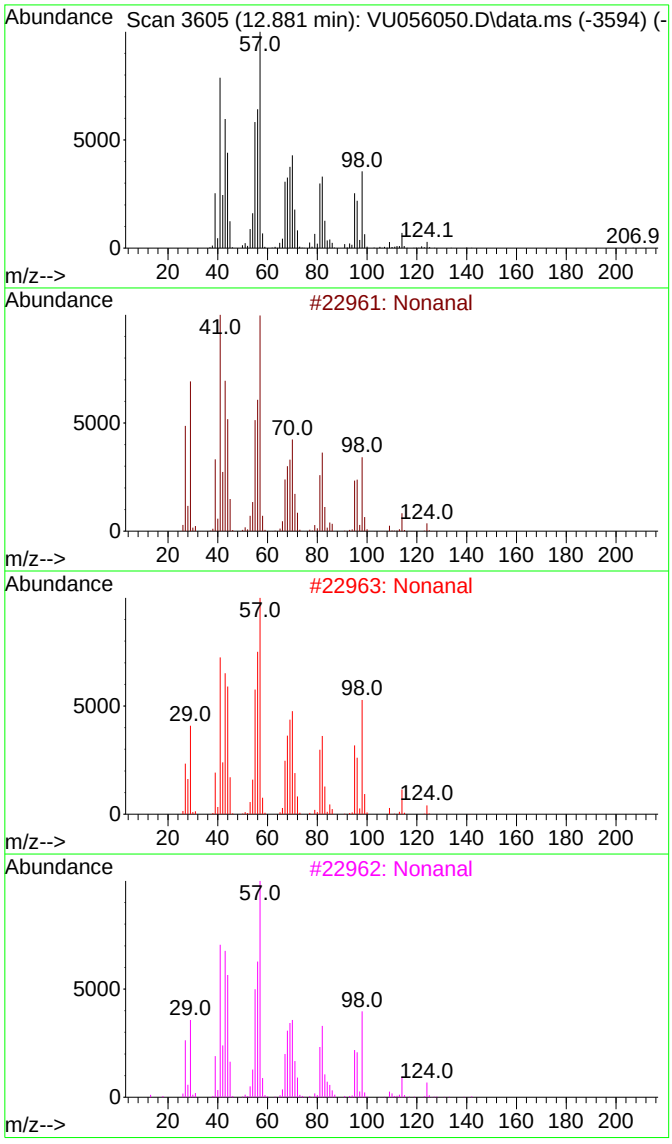
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

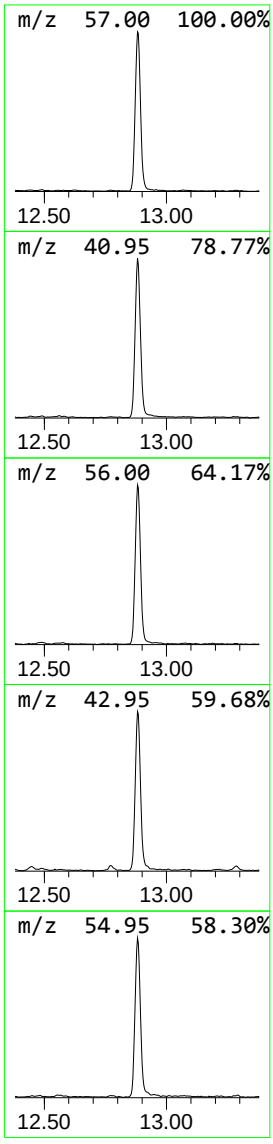
****

Peak Number 8 Nonanal Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.881	5.72 ug/L	1194600	1,4-Dichlorobenzene-d4	11.811

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	Heptane, 2-chloro-	134	C7H15Cl	001001-89-4	27
5	Cyclopentane, 1,2-dimethyl-	98	C7H14	002452-99-5	27





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU110123\
Data File : VU056050.D
Acq On : 01 Nov 2023 19:31
Operator : MD/SY
Sample : 05052-04
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 21 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	1.0	ug/L	171719	1	6.248	897147	5.0
2-Buten-1-ol	4.444	0.8	ug/L	142464	1	6.248	897147	5.0
Hexanal	8.785	0.8	ug/L	182478	2	9.415	1093340	5.0
Heptanal	10.341	0.7	ug/L	159018	2	9.415	1093340	5.0
Octanal	11.685	2.6	ug/L	554663	3	11.811	1045060	5.0
1-Hexanol, 2-et...	12.061	0.8	ug/L	167785	3	11.811	1045060	5.0
Nonanal	12.881	5.7	ug/L	1194600	3	11.811	1045060	5.0