LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

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_V\Method\SFAMVTR061522WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VV026332.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.320	78	87	101	rBV	99414	110771	6.61%	1.128%
2	1.401	104	112	140	rBV	128449	256900	15.33%	2.615%
3	1.581	160	168	182	rVB	93717	112950	6.74%	1.150%
4	2.028	300	307	314	rBV	16337	20698	1.24%	0.211%
5	2.118	326	335	348	rVB2	202161	305513	18.23%	3.110%
6	2.211	350	364	410	rBV2	125993	567963	33.89%	5.781%
7	2.973	588	601	621	rBV3	16578	39016	2.33%	0.397%
8	3.719	815	833	866	rBV2	57039	176791	10.55%	1.800%
9	3.931	883	899	956	rBV3	66582	336452	20.08%	3.425%
10	4.362	1016	1033	1060	rBV2	115263	287568	17.16%	2.927%
11	5.056	1233	1249	1286	rBV2	248277	631793	37.70%	6.431%
12	5.539	1385	1399	1414	rBV	90108	222766	13.29%	2.268%
13	5.622	1414	1425	1464	rVB	269158	574124	34.26%	5.844%
14	5.918	1503	1517	1543	rBV	852699	1675693	100.00%	17.057%
15	6.027	1543	1551	1554	rVV4	13183	21087	1.26%	0.215%
16	6.076	1555	1566	1594	rVB	149113	330945	19.75%	3.369%
17	6.294	1625	1634	1670	rVB3	28076	72144	4.31%	0.734%
18	6.950	1826	1838	1843	rBV4	16092	27680	1.65%	0.282%
19	6.992	1843	1851	1870	rVB2	58448	112266	6.70%	1.143%
20	7.140	1885	1897	1911	rVB6	8306	16959	1.01%	0.173%
21	7.320	1934	1953	1968	rBV	296473	544456	32.49%	5.542%
22	7.394	1969	1976	1998	rVB2	27792	57314	3.42%	0.583%
23	7.629	2038	2049	2067	rBV2	32019	60845	3.63%	0.619%
24	7.979	2151	2158	2171	rVB3	18641	32692	1.95%	0.333%
25	8.095	2183	2194	2231	rBV2	195243	427388	25.51%	4.350%
26	8.243	2231	2240	2269	rVB2	56153	108704	6.49%	1.106%
27	8.725	2381	2390	2407	rBV	33786	61455	3.67%	0.626%
28	8.854	2412	2430	2459	rBV	373061	622614	37.16%	6.338%
29	9.143	2508	2520	2530	rBV2	17413	29660	1.77%	0.302%
30	9.548	2637	2646	2655	rBV3	11101	19059	1.14%	0.194%
31	9.603	2655	2663	2675	rVB2	16683	27066	1.62%	0.276%
32	10.217	2838	2854	2866	rBV	88791	141664	8.45%	1.442%
33	10.375	2884	2903	2919	rBV5	22098	49572	2.96%	0.505%
34	10.510	2936	2945	2951	rBV2	14918	22865	1.36%	0.233%
35	10.921	3063	3073	3095	rBV	40309	79753	4.76%	0.812%
36	11.114	3124	3133	3140	rBV8	10639	21045	1.26%	0.214%

LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

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_V\Method\SFAMVTR061522WMA.M
Title : TRACE VOA SFAM1.0

37	11.246	3164	3174	3197	rBV	344509	534842	31.92%	5.444%
38	11.526	3248	3261	3279	rBV	335583	584951	34.91%	5.954%
39	11.622	3282	3291	3312	rVB	294470	498245	29.73%	5.072%

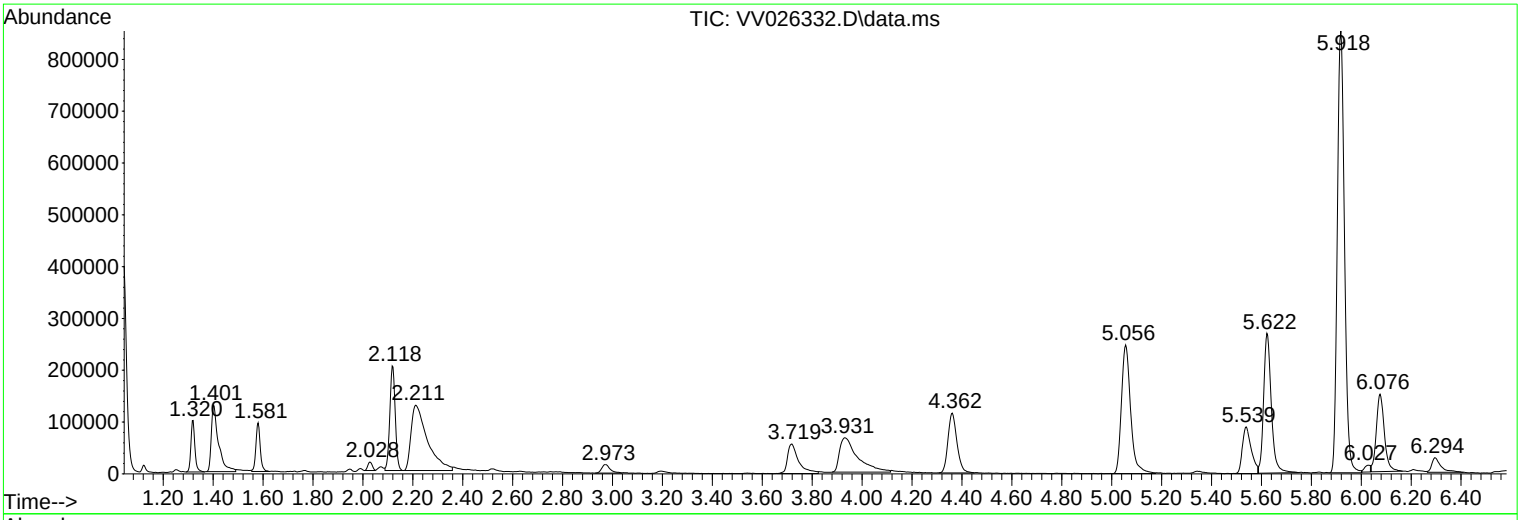
Sum of corrected areas: 9824269

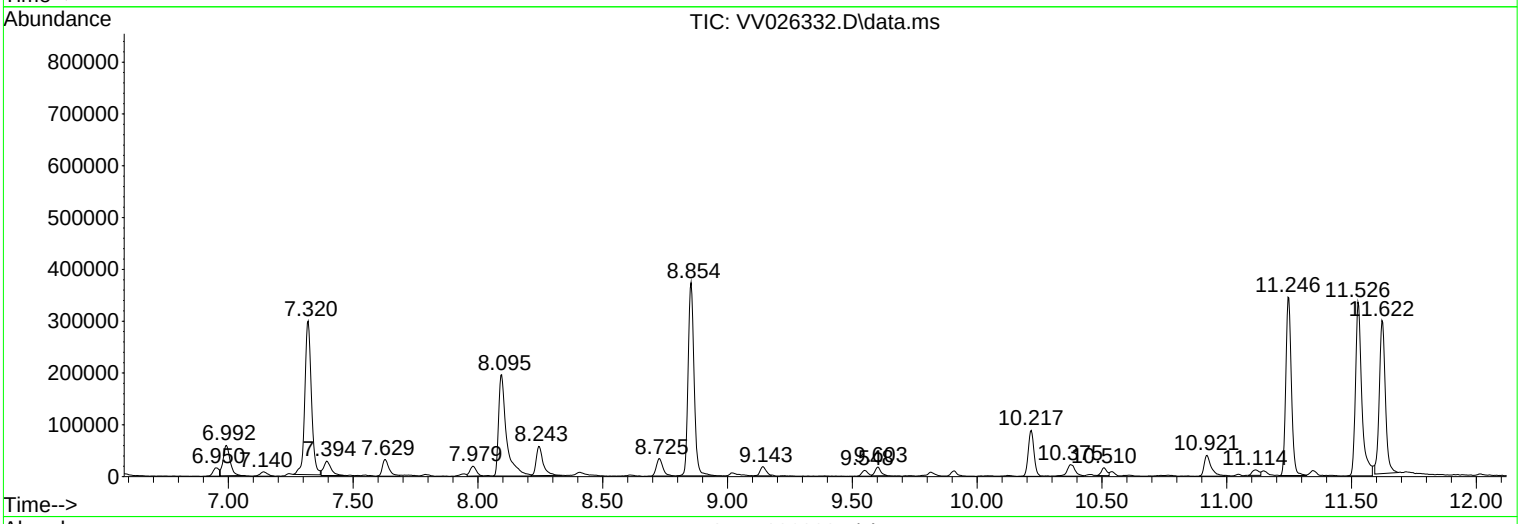
Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

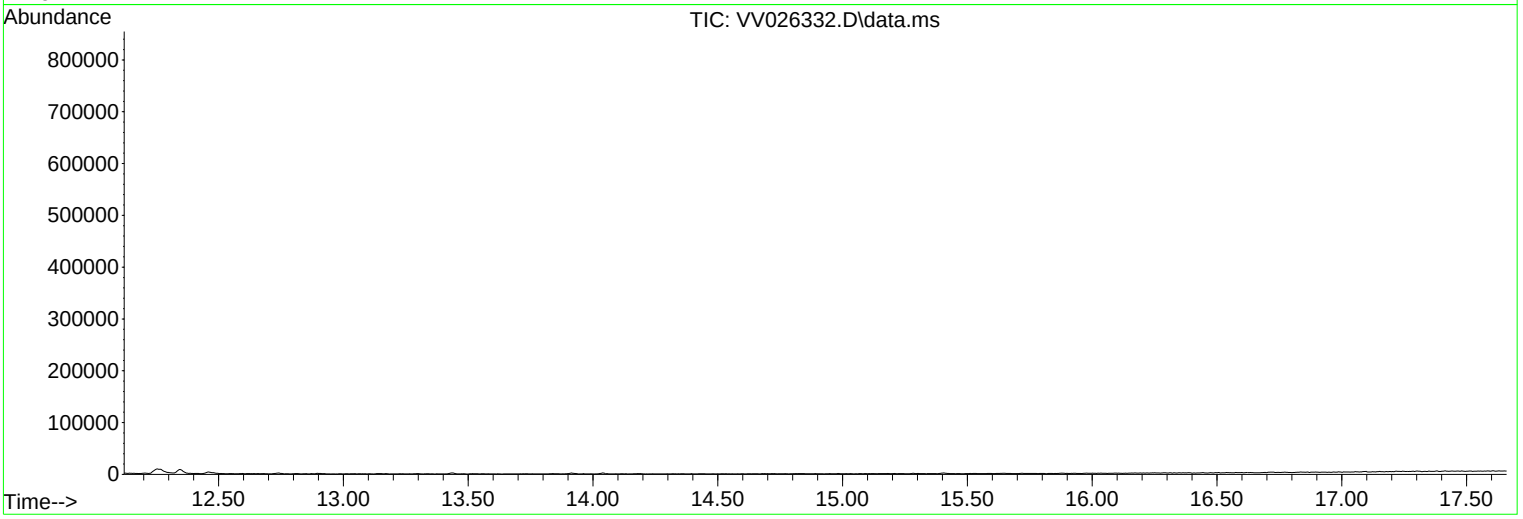
Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

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







Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

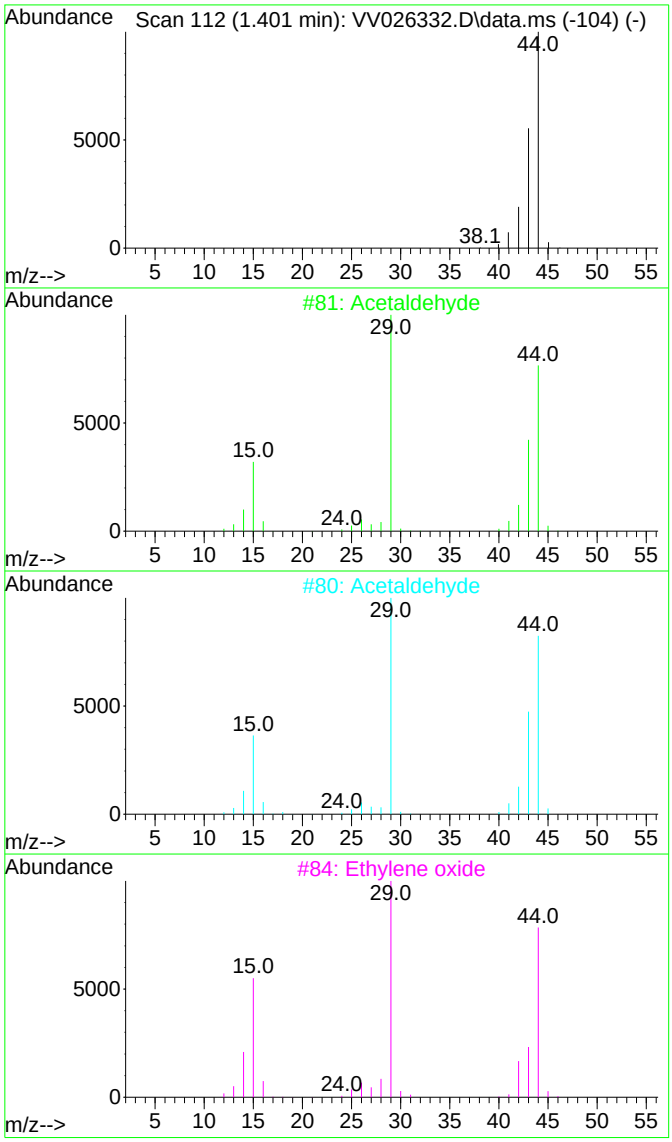
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

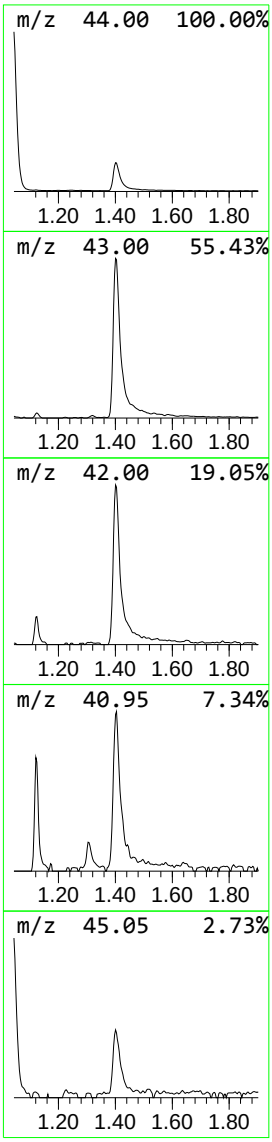
****

Peak Number 1 Acetaldehyde Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.401	2.24 ug/L	256900	1,4-Difluorobenzene	5.622

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	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





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

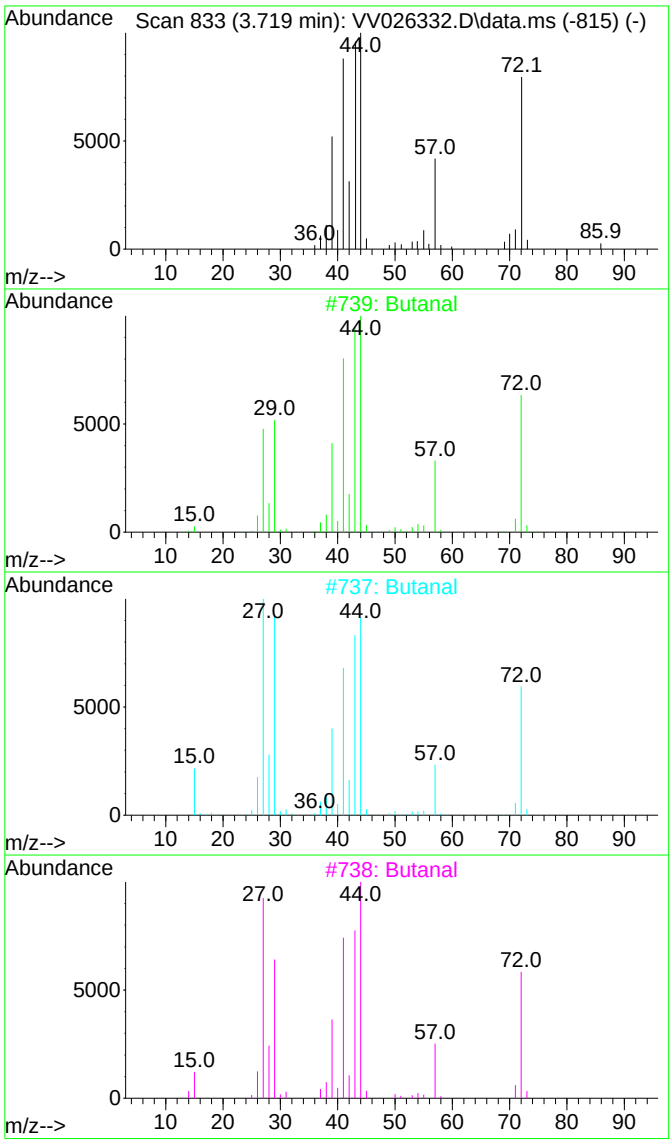
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

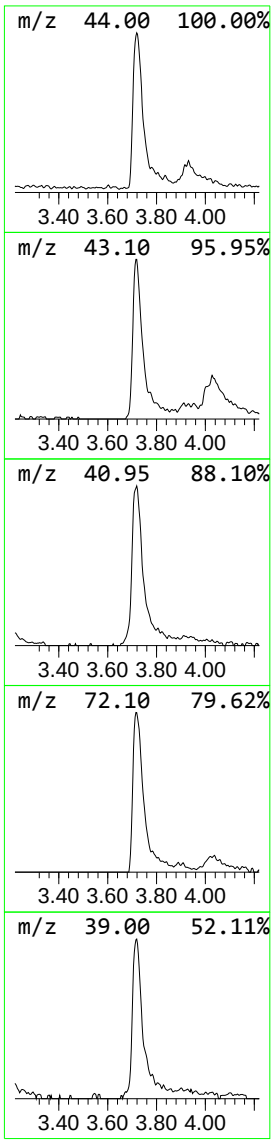
****

Peak Number 2 Butanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.719	1.54 ug/L	176791	1,4-Difluorobenzene	5.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butanal	72	C4H8O	000123-72-8	91
2	Butanal	72	C4H8O	000123-72-8	87
3	Butanal	72	C4H8O	000123-72-8	72
4	Butanal	72	C4H8O	000123-72-8	59
5	Butanal	72	C4H8O	000123-72-8	59





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

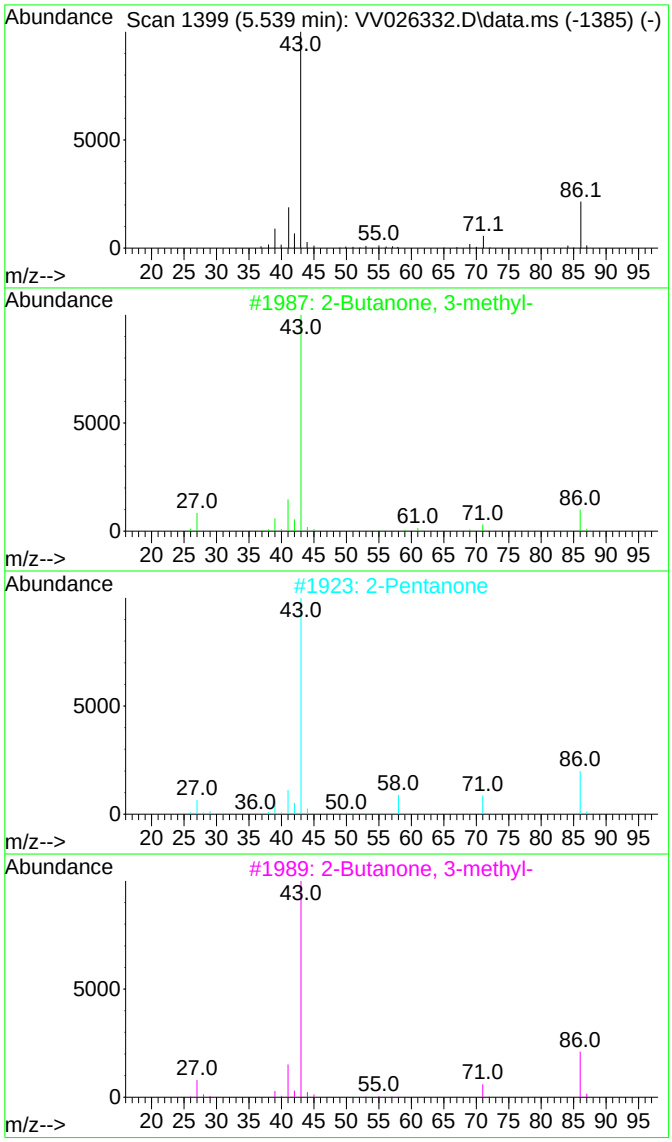
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

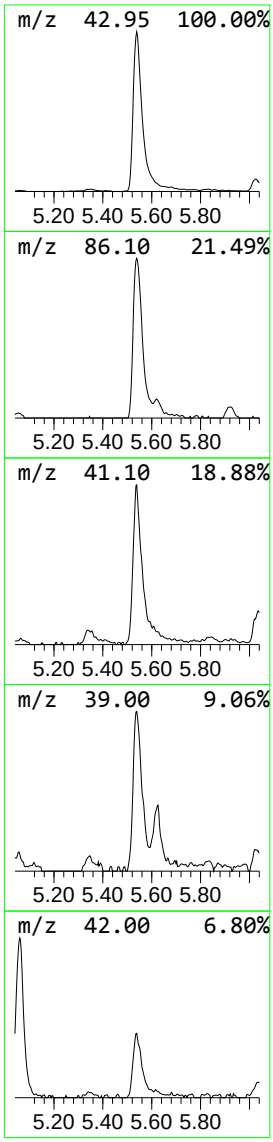
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Butanone, 3-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.539	1.94 ug/L	222766	1,4-Difluorobenzene	5.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	72
2	2-Pentanone	86	C5H10O	000107-87-9	64
3	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
4	2-Butanone, 3-methyl-	86	C5H10O	000563-80-4	59
5	2-Pentanone	86	C5H10O	000107-87-9	53





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

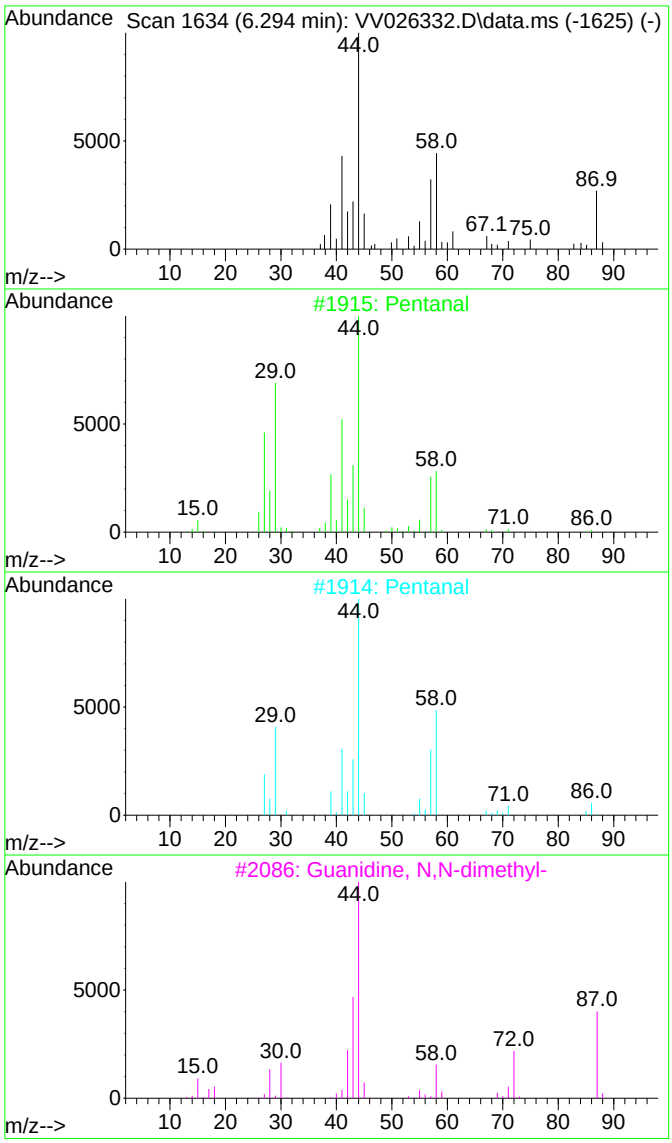
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

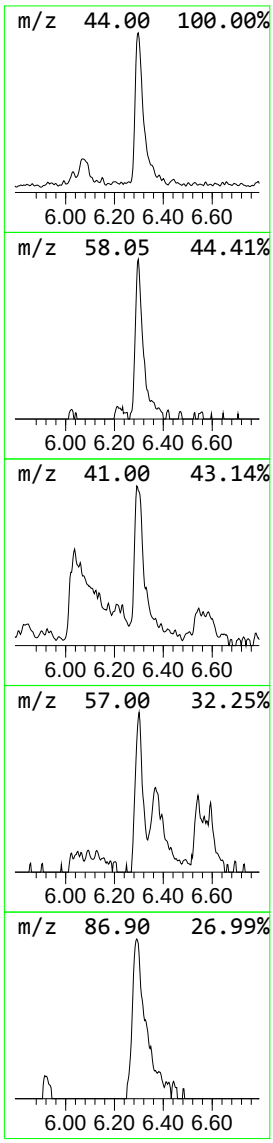
****

Peak Number 4 Pentanal Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.294	0.63 ug/L	72144	1,4-Difluorobenzene	5.622

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal	86	C5H10O	000110-62-3	64
2	Pentanal	86	C5H10O	000110-62-3	64
3	Guanidine, N,N-dimethyl-	87	C3H9N3	006145-42-2	53
4	Butanal, 3-methyl-	86	C5H10O	000590-86-3	50
5	Pentanal	86	C5H10O	000110-62-3	50





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

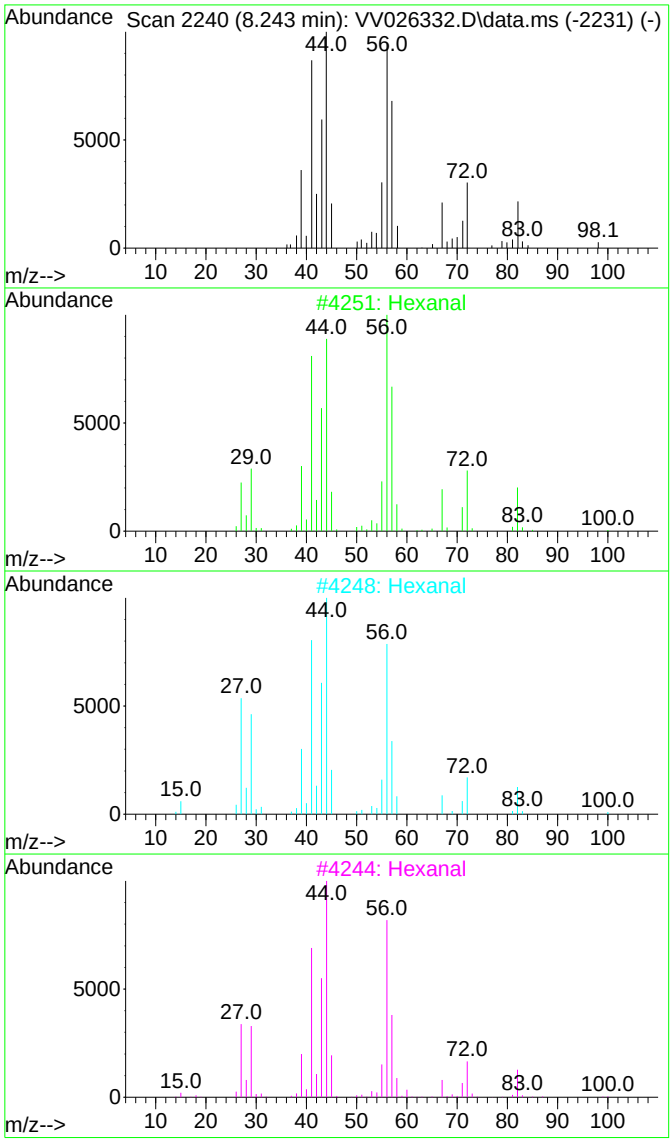
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

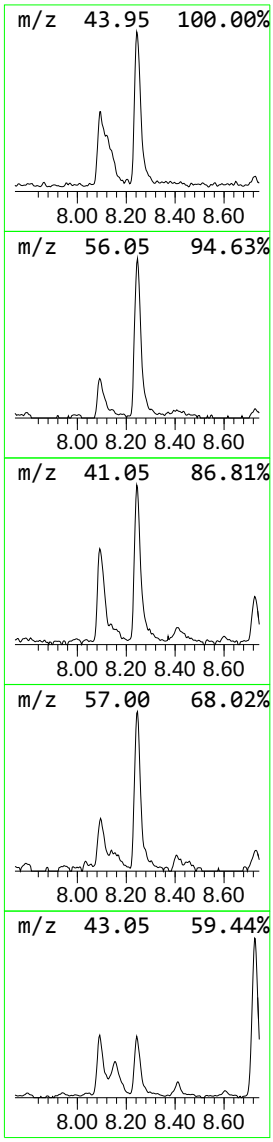
****

Peak Number 6 Hexanal Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.243	0.87 ug/L	108704	Chlorobenzene-d5	8.854

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal	100	C6H12O	000066-25-1	90
2	Hexanal	100	C6H12O	000066-25-1	78
3	Hexanal	100	C6H12O	000066-25-1	78
4	Hexanal	100	C6H12O	000066-25-1	72
5	Hexanal	100	C6H12O	000066-25-1	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

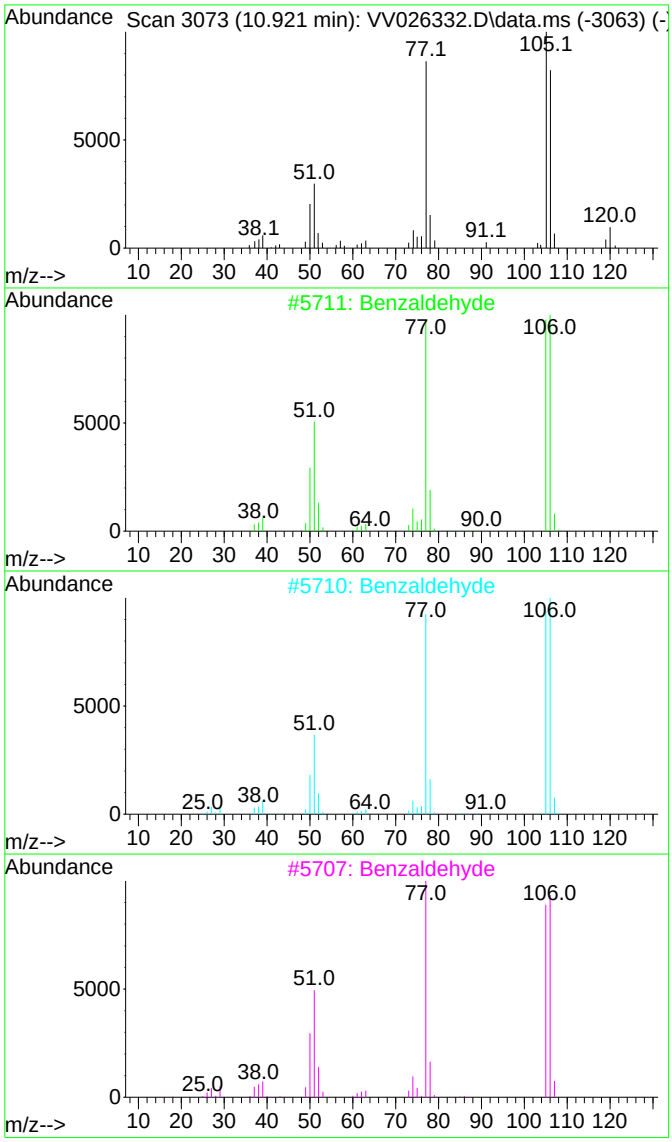
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

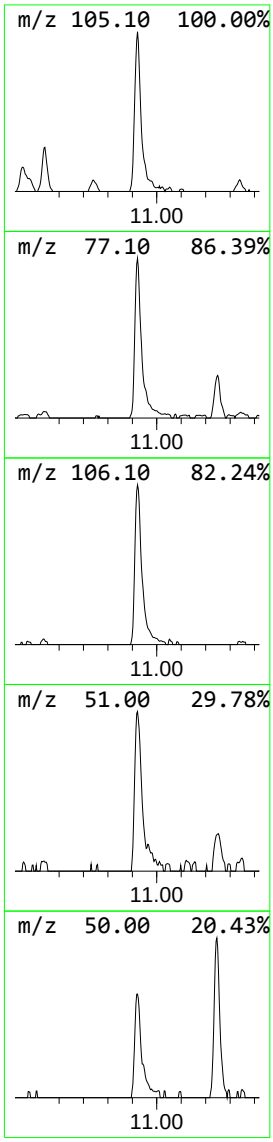
****

Peak Number 7 Benzaldehyde Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.921	0.75 ug/L	79753	1,4-Dichlorobenzene-d4	11.249

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzaldehyde	106	C7H6O	000100-52-7	95
2	Benzaldehyde	106	C7H6O	000100-52-7	93
3	Benzaldehyde	106	C7H6O	000100-52-7	93
4	Benzaldehyde	106	C7H6O	000100-52-7	93
5	Benzaldehyde	106	C7H6O	000100-52-7	91





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

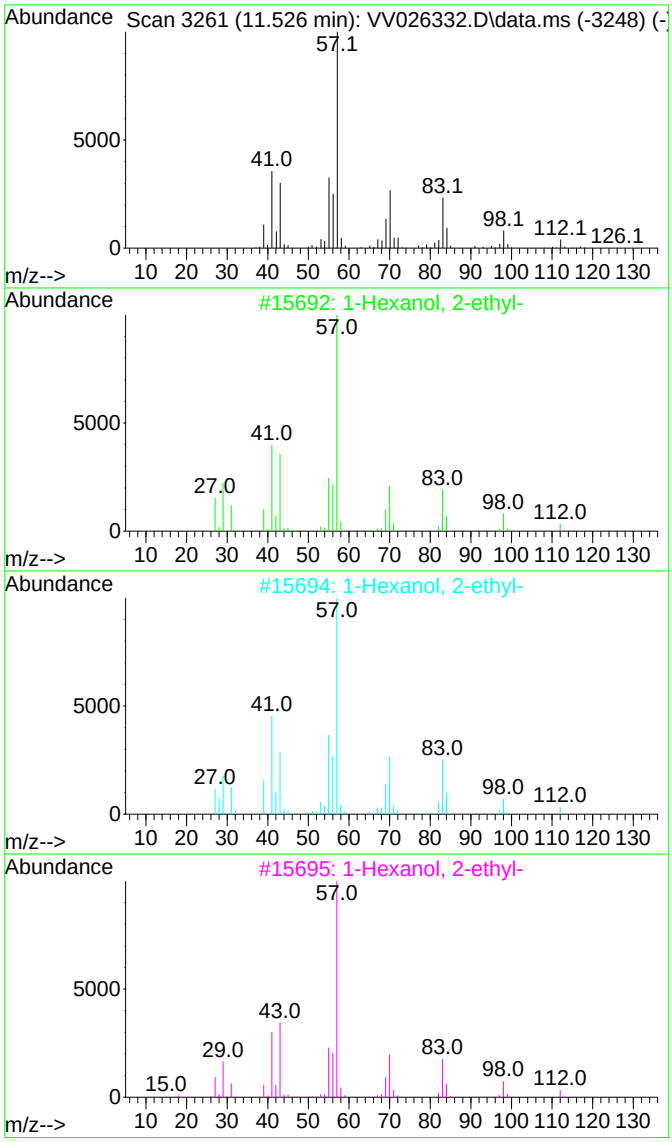
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.M
Quant Title : TRACE VOA SFAM1.0

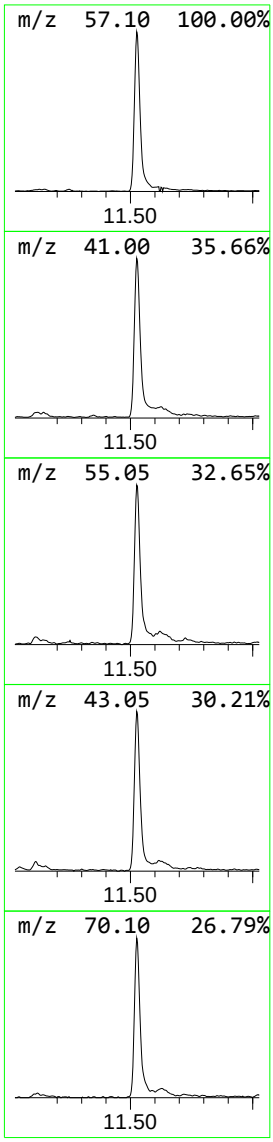
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.526	5.47 ug/L	584951	1,4-Dichlorobenzene-d4	11.249

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





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV061622\
Data File : VV026332.D
Acq On : 16 Jun 2022 14:35
Operator : SY/MD
Sample : N3275-05
Misc : 25mL/MSVOA_V/WATER
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0BD7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR061522WMA.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	1.401	2.2	ug/L	256900	1	5.622	574124	5.0
Butanal	3.719	1.5	ug/L	176791	1	5.622	574124	5.0
2-Butanone, 3-m...	5.539	1.9	ug/L	222766	1	5.622	574124	5.0
Pentanal	6.294	0.6	ug/L	72144	1	5.622	574124	5.0
Hexanal	8.243	0.9	ug/L	108704	2	8.854	622614	5.0
Benzaldehyde	10.921	0.8	ug/L	79753	3	11.249	534842	5.0
1-Hexanol, 2-et...	11.526	5.5	ug/L	584951	3	11.249	534842	5.0