

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
 Data File : VV032441.D
 Acq On : 17 Oct 2023 13:29
 Operator : SY/MD
 Sample : 04903-15
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AF8

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\SFAMVTR092923WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VV032441.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.105	14	20	32	rVB2	7452	12797	2.84%	0.299%
2	1.278	67	74	91	rVB	54041	60434	13.41%	1.411%
3	1.362	91	100	113	rBV3	10668	25841	5.74%	0.604%
4	1.532	146	153	167	rVB	50001	58254	12.93%	1.361%
5	2.059	306	317	331	rBV	82501	123531	27.42%	2.885%
6	2.706	503	518	528	rBV5	4272	10270	2.28%	0.240%
7	2.892	563	576	592	rBV3	14960	35403	7.86%	0.827%
8	3.818	854	864	892	rBV2	35193	133613	29.66%	3.121%
9	4.272	980	1005	1025	rBV4	104222	372070	82.59%	8.690%
10	4.963	1204	1220	1238	rBV2	135796	350151	77.72%	8.178%
11	5.246	1297	1308	1325	rBV4	12788	31815	7.06%	0.743%
12	5.426	1352	1364	1385	rBV3	12157	32721	7.26%	0.764%
13	5.538	1388	1399	1415	rBV	112080	232890	51.70%	5.439%
14	5.834	1482	1491	1496	rBV6	2677	4767	1.06%	0.111%
15	5.992	1528	1540	1553	rBV	80487	173414	38.49%	4.050%
16	6.436	1662	1678	1710	rBV2	85420	187988	41.73%	4.391%
17	6.918	1814	1828	1855	rBV2	35622	79977	17.75%	1.868%
18	7.188	1902	1912	1920	rBV3	9192	19258	4.27%	0.450%
19	7.246	1920	1930	1951	rVV	150423	283967	63.03%	6.632%
20	7.374	1962	1970	1987	rVB	11347	24655	5.47%	0.576%
21	7.561	2017	2028	2034	rBV2	22008	37053	8.22%	0.865%
22	7.879	2116	2127	2143	rBV2	24287	47687	10.59%	1.114%
23	8.034	2163	2175	2209	rBV	192079	450504	100.00%	10.522%
24	8.181	2210	2221	2245	rVB	82282	167308	37.14%	3.908%
25	8.789	2400	2410	2433	rBV	185381	324874	72.11%	7.588%
26	8.956	2455	2462	2473	rVB2	4585	7270	1.61%	0.170%
27	9.082	2490	2501	2516	rVB3	7952	15506	3.44%	0.362%
28	9.487	2617	2627	2637	rBV4	4931	9212	2.04%	0.215%
29	9.670	2675	2684	2697	rBV2	16146	28250	6.27%	0.660%
30	10.159	2824	2836	2852	rBV	71345	118136	26.22%	2.759%
31	10.329	2879	2889	2900	rVB2	49425	84113	18.67%	1.965%
32	10.390	2901	2908	2912	rBV3	5334	6682	1.48%	0.156%
33	10.451	2919	2927	2943	rVB2	18470	31441	6.98%	0.734%
34	10.676	2988	2997	3005	rBV10	3081	4950	1.10%	0.116%
35	10.857	3045	3053	3064	rBV2	7095	11611	2.58%	0.271%
36	11.188	3146	3156	3175	rBV	192651	307152	68.18%	7.174%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

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\SFAMVTR092923WMA.M
Title : TRACE VOA SFAM1.0

37	11.496	3237	3252	3255	rBV6	12117	21684	4.81%	0.506%
38	11.564	3263	3273	3293	rVB	176524	289371	64.23%	6.758%
39	12.201	3460	3471	3483	rVB	25219	40450	8.98%	0.945%
40	12.291	3494	3499	3510	rBV9	4965	7730	1.72%	0.181%
41	13.448	3850	3859	3868	rBV2	5677	8905	1.98%	0.208%
42	13.988	4020	4027	4035	rVB2	4944	7930	1.76%	0.185%

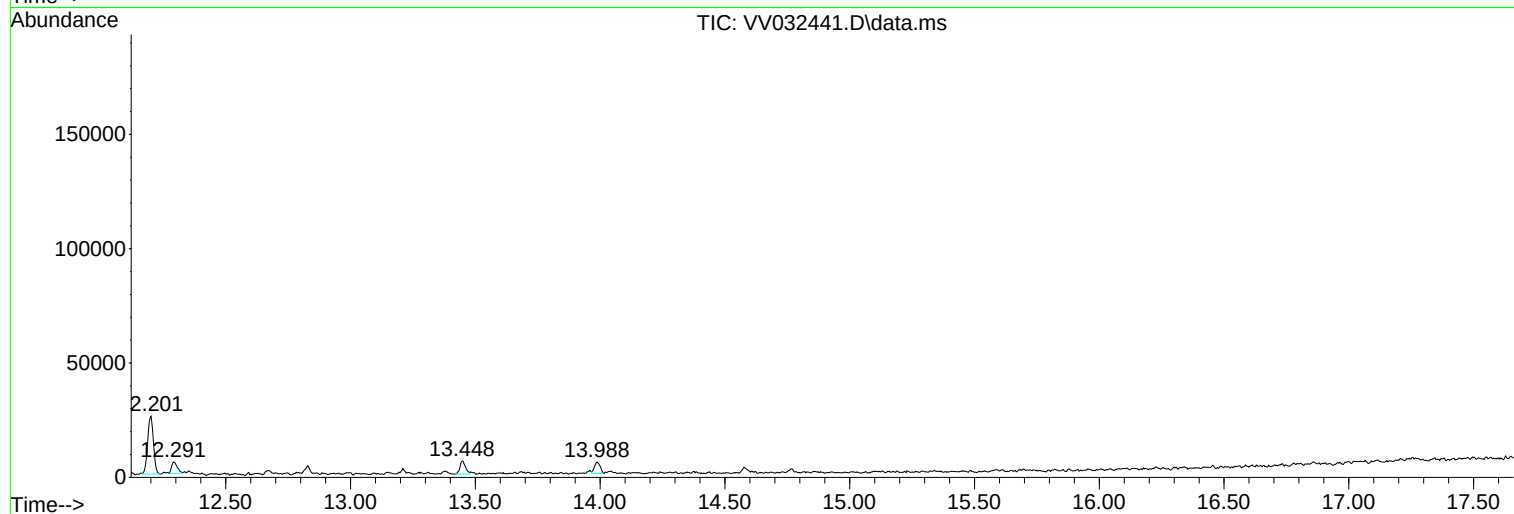
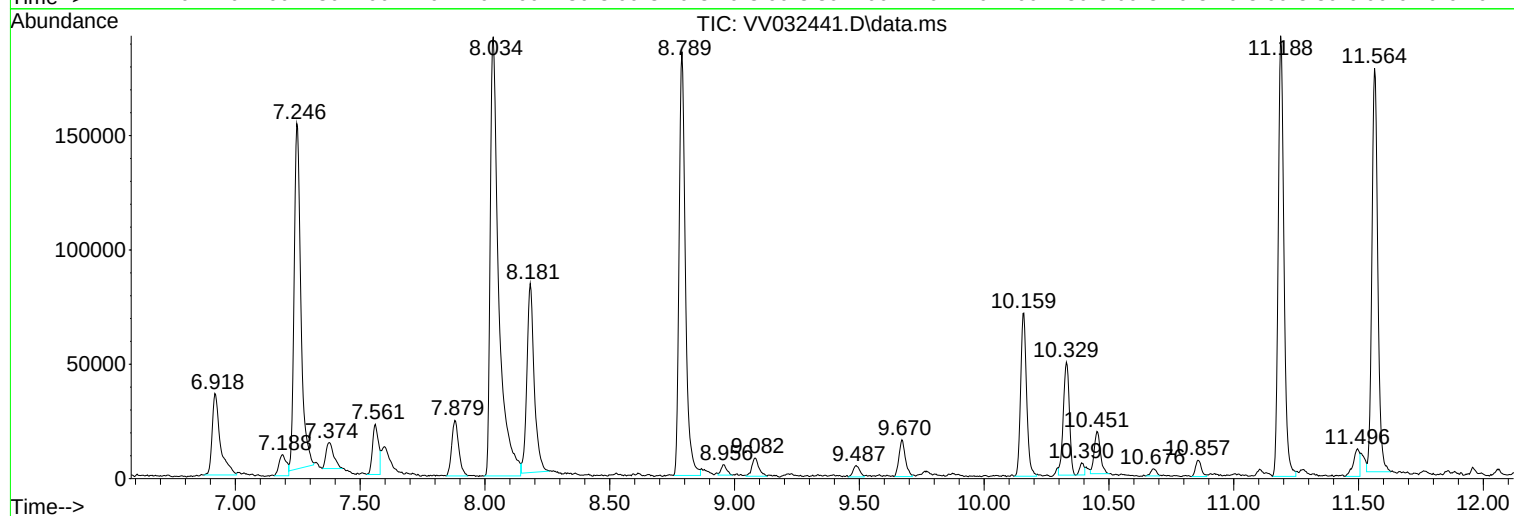
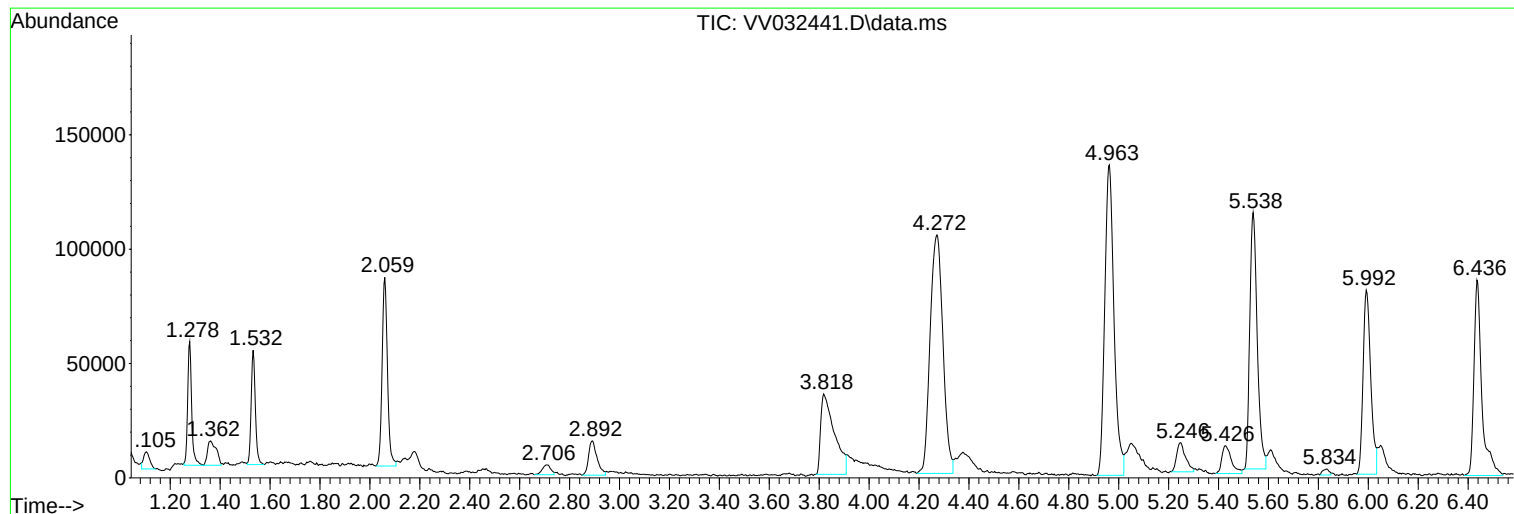
Sum of corrected areas: 4281635

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.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\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

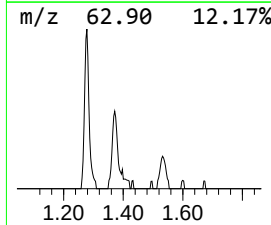
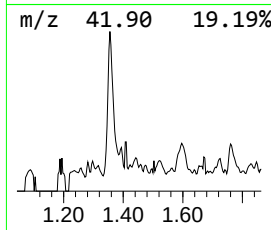
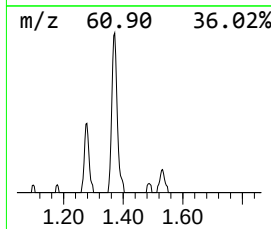
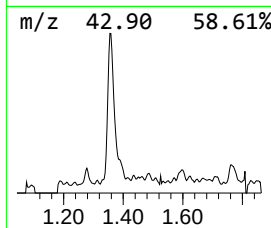
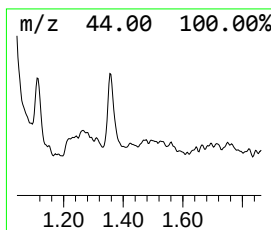
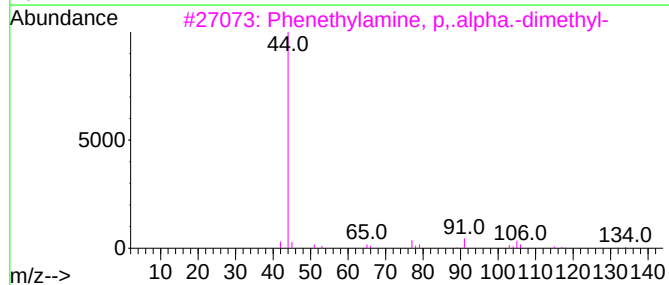
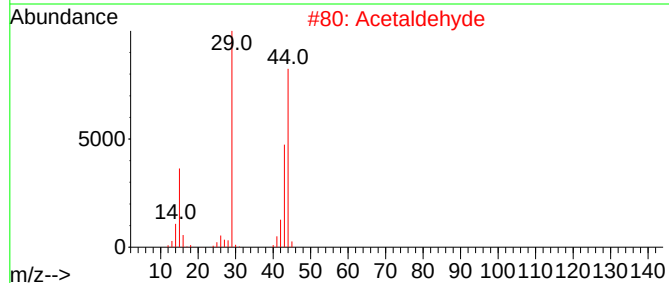
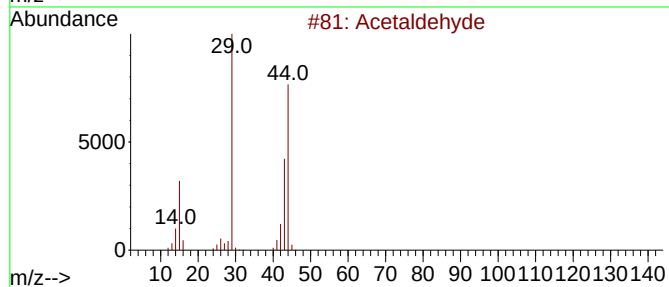
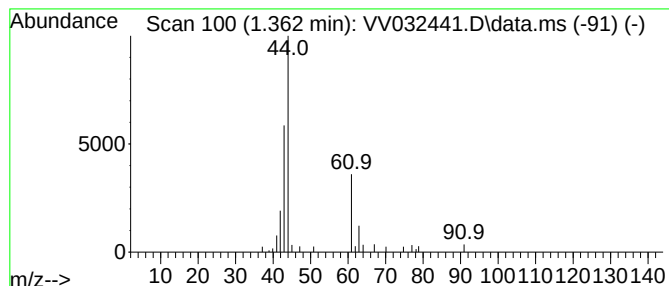
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.362	0.55 ug/L	25841	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetaldehyde	44	C2H4O	000075-07-0	40
2			Acetaldehyde	44	C2H4O	000075-07-0	40
3			Phenethylamine, p,.alpha.-dimethyl-	149	C10H15N	000064-11-9	25
4			Ortetamine	149	C10H15N	005580-32-5	23
5			Benzenemethanol, .alpha.-[(methy...	151	C9H13NO	006589-55-5	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

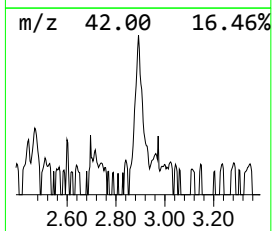
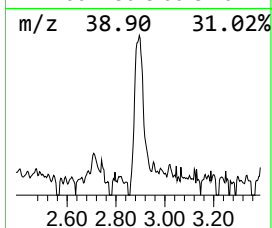
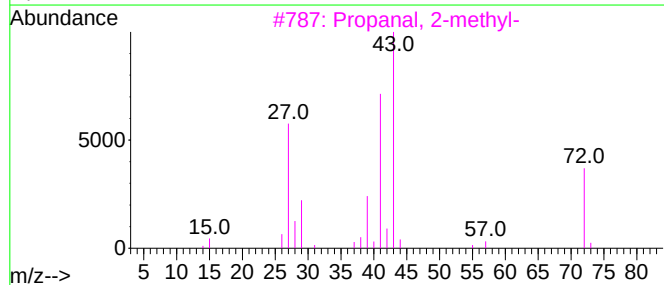
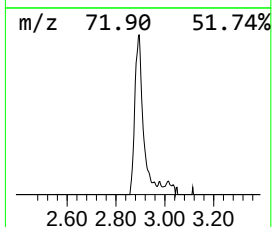
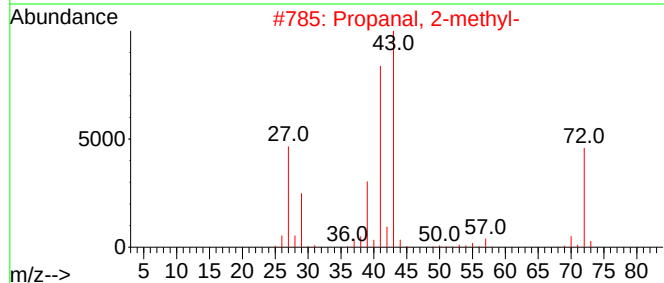
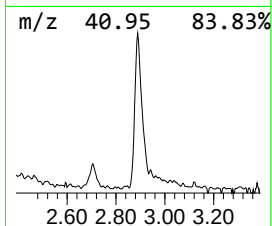
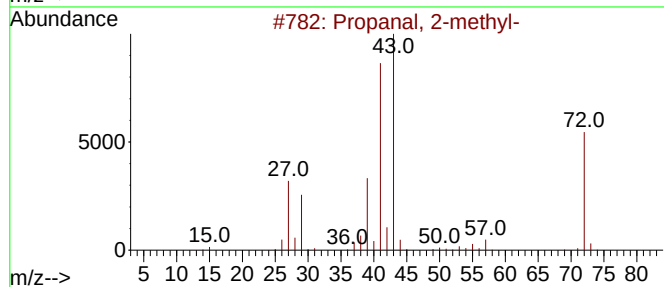
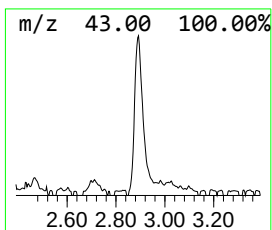
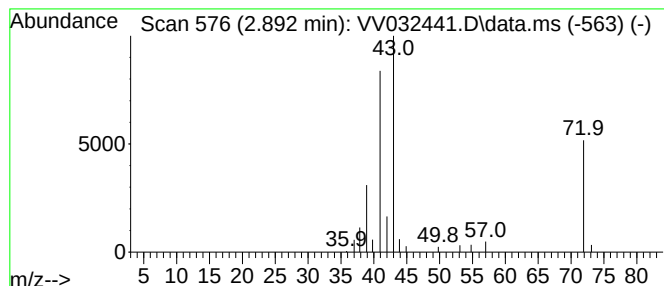
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propanal, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.892	0.76 ug/L	35403	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanal, 2-methyl-			72	C4H8O	000078-84-2	91
2	Propanal, 2-methyl-			72	C4H8O	000078-84-2	90
3	Propanal, 2-methyl-			72	C4H8O	000078-84-2	86
4	Propanal, 2-methyl-			72	C4H8O	000078-84-2	72
5	Butanal			72	C4H8O	000123-72-8	58



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

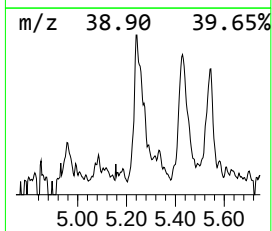
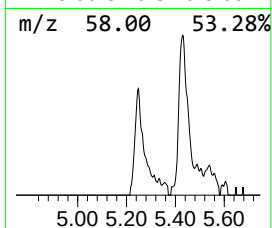
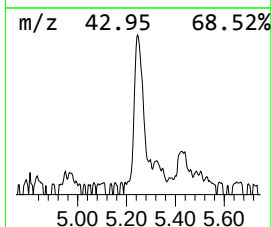
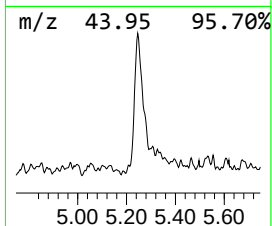
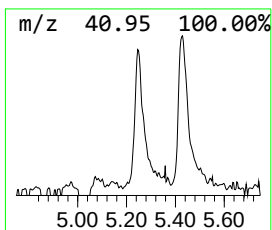
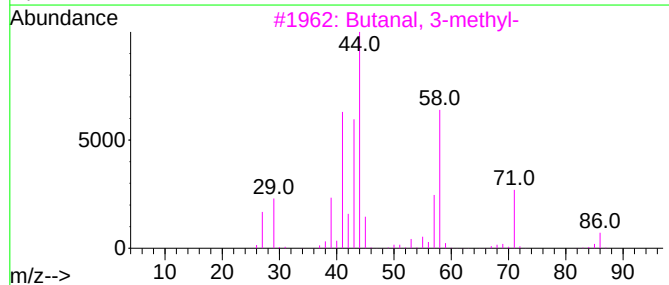
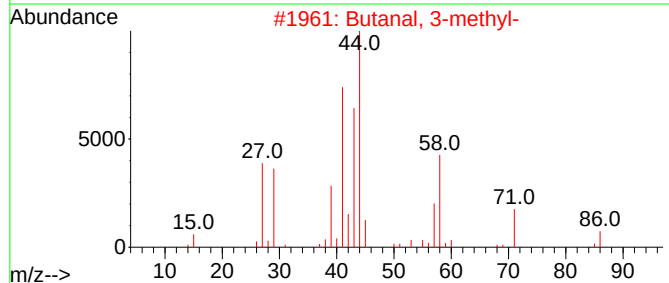
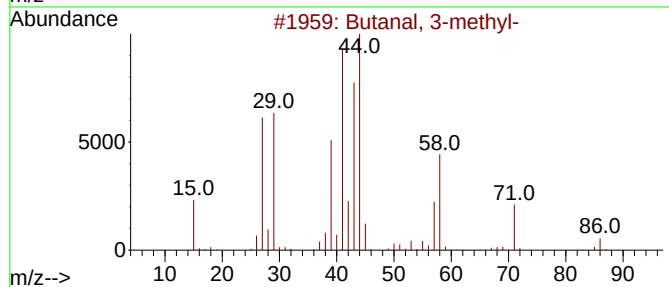
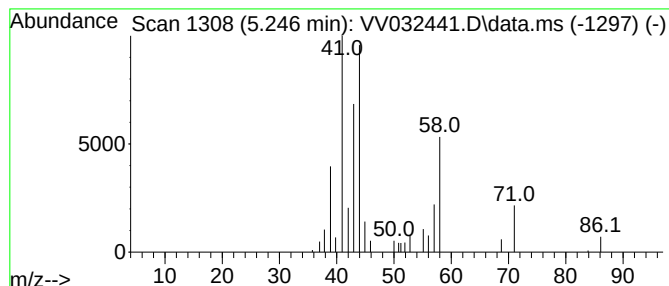
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Butanal, 3-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.246	0.68 ug/L	31815	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 3-methyl-	86	C5H10O	000590-86-3	87
2			Butanal, 3-methyl-	86	C5H10O	000590-86-3	74
3			Butanal, 3-methyl-	86	C5H10O	000590-86-3	58
4			Butanal, 3-methyl-	86	C5H10O	000590-86-3	49
5			Pentanal	86	C5H10O	000110-62-3	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

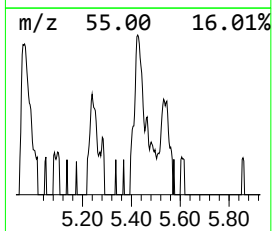
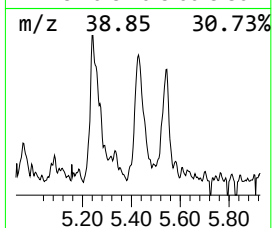
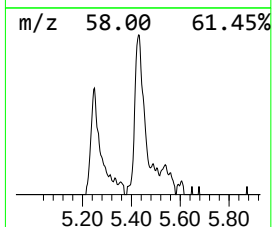
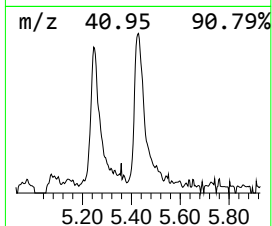
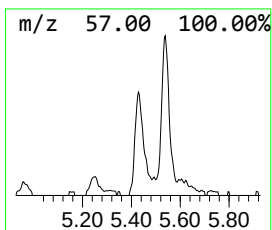
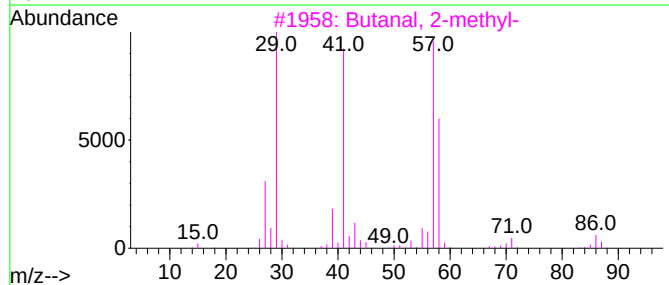
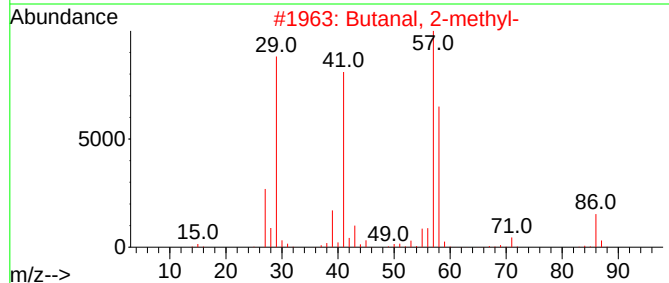
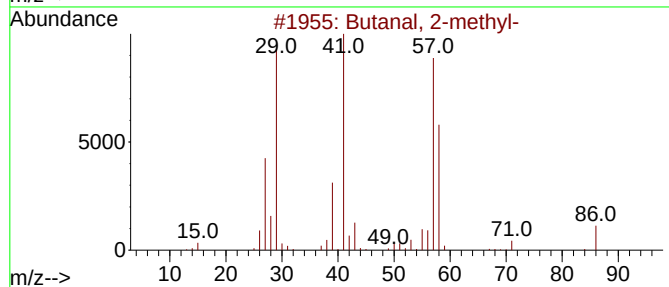
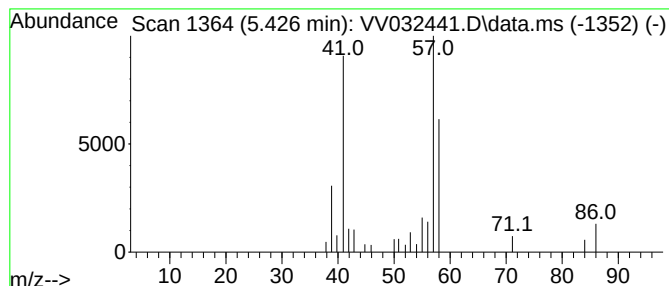
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 Butanal, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.426	0.70 ug/L	32721	1,4-Difluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal, 2-methyl-	86	C5H10O	000096-17-3	90
2			Butanal, 2-methyl-	86	C5H10O	000096-17-3	80
3			Butanal, 2-methyl-	86	C5H10O	000096-17-3	78
4			2-Penten-1-ol, (E)-	86	C5H10O	001576-96-1	35
5			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	32



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

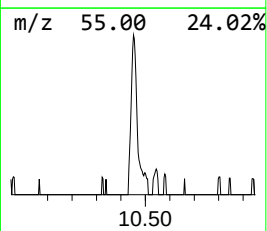
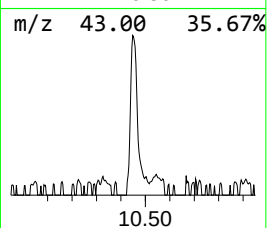
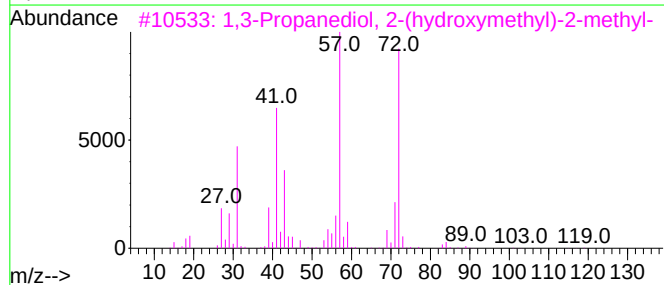
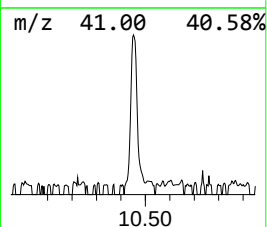
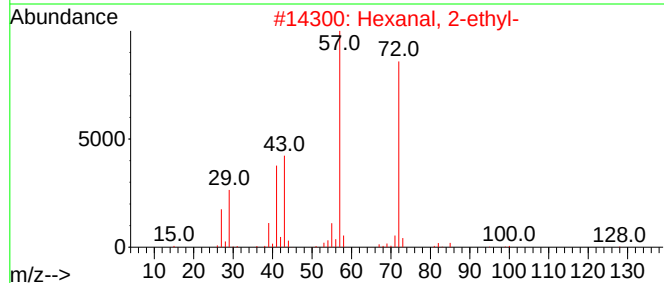
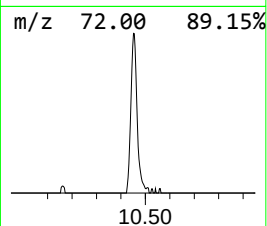
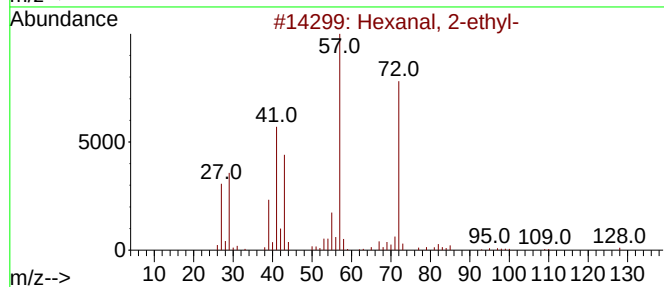
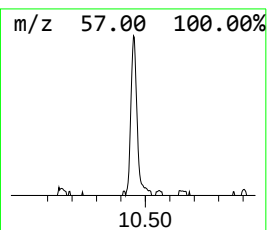
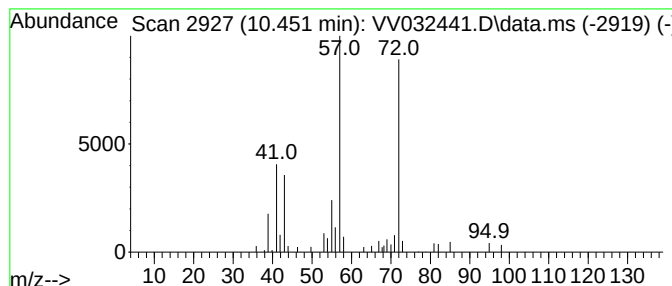
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 8 Hexanal, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.451	0.51 ug/L	31441	1,4-Dichlorobenzene-d4	11.188

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	72
2			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	64
3			1,3-Propanediol, 2-(hydroxymethy...	120	C5H12O3	000077-85-0	64
4			1,3-Cyclobutanediol, 2,2,4,4-tet...	144	C8H16O2	003010-96-6	59
5			Hexanal, 2-ethyl-	128	C8H16O	000123-05-7	56



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV101723\
Data File : VV032441.D
Acq On : 17 Oct 2023 13:29
Operator : SY/MD
Sample : 04903-15
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AF8

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR092923WMA.M
Quant Title : TRACE VOA SFAM1.0

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.362	0.6	ug/L	25841	1	5.538	232890	5.0
Propanal, 2-met...	2.892	0.8	ug/L	35403	1	5.538	232890	5.0
Butanal, 3-methyl-	5.246	0.7	ug/L	31815	1	5.538	232890	5.0
Butanal, 2-methyl-	5.426	0.7	ug/L	32721	1	5.538	232890	5.0
Hexanal, 2-ethyl-	10.451	0.5	ug/L	31441	3	11.188	307152	5.0