LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

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\SFAMVTR011224WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VV033650.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.082	7	13	28	rVB2	25682	29884	2.37%	0.430%
2	1.185	38	45	54	rBV	49586	47030	3.73%	0.677%
3	1.275	62	73	82	rBV3	149811	189479	15.04%	2.729%
4	1.529	145	152	162	rVB	37902	44328	3.52%	0.639%
5	1.590	165	171	183	rVB	26229	32654	2.59%	0.470%
6	1.761	219	224	235	rBV5	10167	14054	1.12%	0.202%
7	2.053	307	315	336	rVB	68106	106608	8.46%	1.536%
8	2.510	450	457	473	rVB5	18591	43612	3.46%	0.628%
9	2.683	501	511	524	rBV4	15337	29764	2.36%	0.429%
10	3.108	630	643	654	rBV2	10618	20369	1.62%	0.293%
11	3.178	655	665	687	rVB6	7817	19266	1.53%	0.278%
12	3.658	798	814	830	rBV2	12402	29885	2.37%	0.430%
13	3.809	847	861	878	rBV	234187	553434	43.94%	7.972%
14	4.249	980	998	1022	rBV	55106	147806	11.73%	2.129%
15	4.574	1084	1099	1113	rBV4	10313	25685	2.04%	0.370%
16	4.664	1115	1127	1149	rVB7	5457	17716	1.41%	0.255%
17	4.953	1201	1217	1228	rBV2	131057	311781	24.75%	4.491%
18	5.133	1263	1273	1288	rVB5	10838	28213	2.24%	0.406%
19	5.230	1291	1303	1315	rBV9	6437	14070	1.12%	0.203%
20	5.532	1386	1397	1436	rBV	130878	286664	22.76%	4.129%
21	5.789	1459	1477	1487	rBV2	5849	14472	1.15%	0.208%
22	5.989	1522	1539	1568	rBV2	74280	187852	14.91%	2.706%
23	6.571	1708	1720	1741	rVB8	5015	14938	1.19%	0.215%
24	6.696	1744	1759	1776	rBV7	6111	18645	1.48%	0.269%
25	6.918	1819	1828	1851	rVB	38849	74029	5.88%	1.066%
26	7.091	1869	1882	1894	rVB6	12756	27087	2.15%	0.390%
27	7.243	1902	1929	1946	rBV	151703	284261	22.57%	4.095%
28	7.558	2009	2027	2044	rBV4	22210	58367	4.63%	0.841%
29	8.037	2158	2176	2193	rBV	135918	283755	22.53%	4.087%
30	8.140	2203	2208	2227	rVB8	18057	41519	3.30%	0.598%
31	8.786	2399	2409	2413	rBV	207145	317901	25.24%	4.579%
32	9.075	2492	2499	2511	rVB2	19155	33988	2.70%	0.490%
33	9.246	2546	2552	2570	rVB2	6847	14653	1.16%	0.211%
34	9.410	2586	2603	2619	rBV2	7844	28440	2.26%	0.410%
35	9.638	2658	2674	2685	rBV7	10470	23369	1.86%	0.337%
36	9.738	2693	2705	2716	rBV7	9650	24513	1.95%	0.353%

LSC Area Percent Report

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Misc : 25.0mL/MSVOA_V/WATER
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MSVOA_V
ClientSampleId :
C0AY0

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\SFAMVTR011224WMA.M
Title : TRACE VOA SFAM1.0

37	9.870	2737	2746	2754	rBV	12992	23440	1.86%	0.338%
38	10.059	2798	2805	2814	rVB8	8249	13570	1.08%	0.195%
39	10.156	2825	2835	2851	rVB2	50693	91742	7.28%	1.321%
40	10.673	2988	2996	3015	rVB2	26485	60080	4.77%	0.865%
41	10.799	3028	3035	3044	rVB2	15459	26516	2.11%	0.382%
42	10.873	3049	3058	3069	rVB5	15055	28237	2.24%	0.407%
43	10.934	3069	3077	3087	rBV	14913	24905	1.98%	0.359%
44	10.992	3087	3095	3100	rBV	40409	58914	4.68%	0.849%
45	11.024	3101	3105	3119	rVB	28506	43060	3.42%	0.620%
46	11.117	3125	3134	3145	rBV	87108	141426	11.23%	2.037%
47	11.207	3146	3162	3181	rVB2	610476	1259585	100.00%	18.143%
48	11.390	3213	3219	3231	rVB8	13664	23674	1.88%	0.341%
49	11.574	3257	3276	3301	rVB3	231087	605766	48.09%	8.726%
50	11.686	3302	3311	3321	rBV10	14342	29969	2.38%	0.432%
51	11.779	3336	3340	3352	rVB10	14287	21044	1.67%	0.303%
52	11.921	3377	3384	3393	rBV6	14844	26065	2.07%	0.375%
53	11.992	3400	3406	3417	rVB8	19038	33105	2.63%	0.477%
54	12.059	3419	3427	3446	rVB10	26389	69483	5.52%	1.001%
55	12.181	3457	3465	3472	rBV6	26092	49235	3.91%	0.709%
56	12.493	3557	3562	3569	rVB2	12117	14440	1.15%	0.208%
57	12.622	3595	3602	3611	rVV2	43078	66632	5.29%	0.960%
58	12.664	3612	3615	3624	rVB4	13150	14393	1.14%	0.207%
59	12.818	3655	3663	3669	rBV5	21599	35482	2.82%	0.511%
60	13.104	3738	3752	3761	rBV3	21661	55198	4.38%	0.795%
61	13.204	3775	3783	3789	rBV5	30764	51170	4.06%	0.737%
62	13.249	3790	3797	3801	rBV3	27788	43818	3.48%	0.631%
63	13.480	3864	3869	3879	rVB5	20783	30708	2.44%	0.442%
64	13.545	3882	3889	3902	rVB5	33601	62527	4.96%	0.901%
65	13.631	3904	3916	3933	rBV10	28178	91482	7.26%	1.318%
66	13.770	3951	3959	3972	rVB10	11746	26066	2.07%	0.375%
67	14.043	4034	4044	4054	rVB7	15723	34575	2.74%	0.498%
68	14.168	4076	4083	4091	rVB	37463	52173	4.14%	0.752%
69	14.236	4095	4104	4112	rVB4	26137	44866	3.56%	0.646%
70	14.377	4140	4148	4159	rVB5	20127	43286	3.44%	0.624%
71	14.512	4183	4190	4197	rBV5	11946	18637	1.48%	0.268%
72	15.104	4366	4374	4384	rBV2	14453	23090	1.83%	0.333%
73	15.274	4415	4427	4444	rVB7	13405	36664	2.91%	0.528%
74	15.381	4446	4460	4473	rBV8	10018	29067	2.31%	0.419%
75	15.528	4501	4506	4516	rVB6	8805	12972	1.03%	0.187%
76	15.602	4523	4529	4534	rBV7	10334	15211	1.21%	0.219%

LSC Area Percent Report

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Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

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\SFAMVTR011224WMA.M
Title : TRACE VOA SFAM1.0

77	15.750	4566	4575	4582	rBV2	26600	43533	3.46%	0.627%
78	15.789	4583	4587	4600	rVB8	16171	26502	2.10%	0.382%

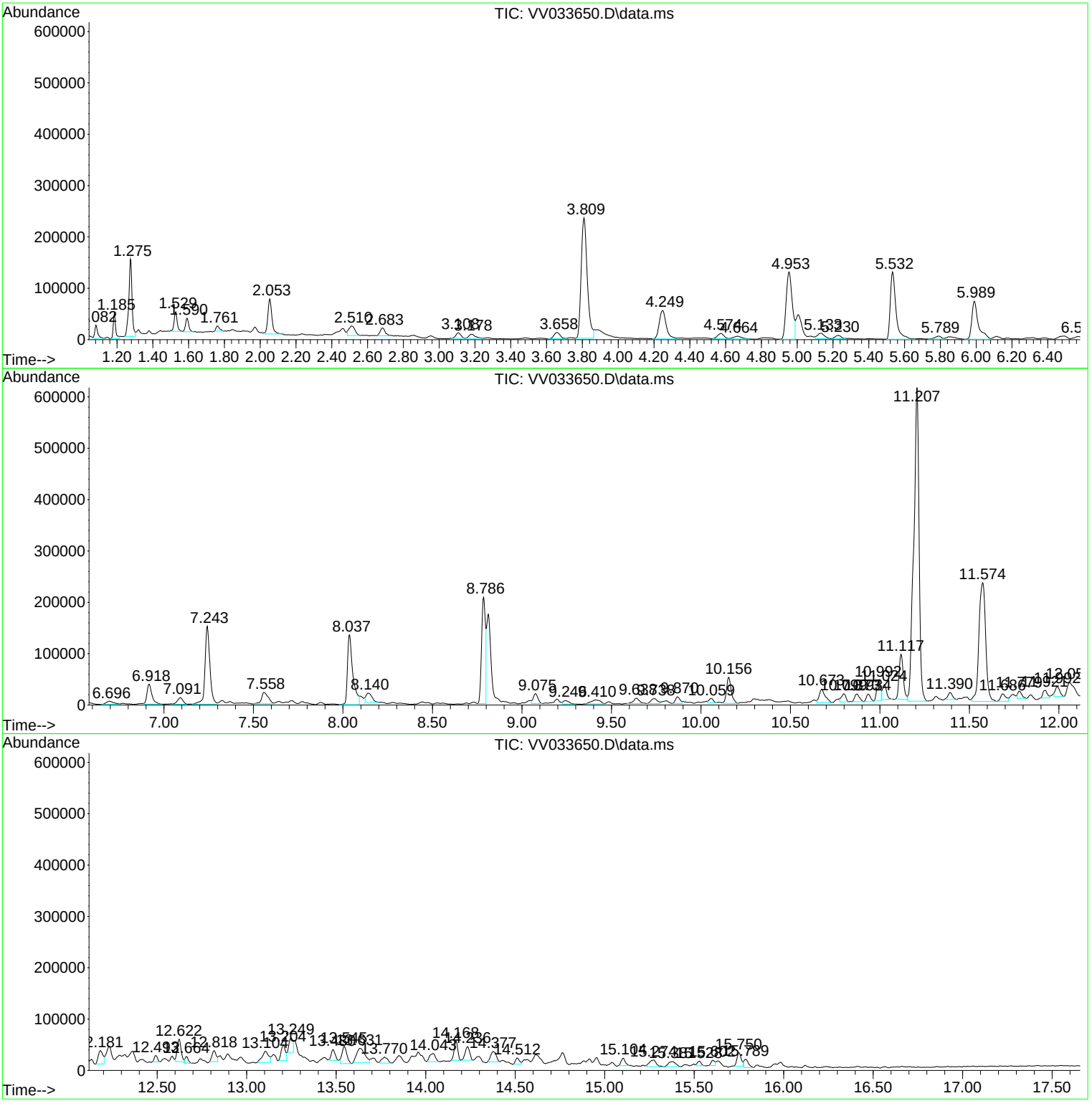
Sum of corrected areas: 6942399

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.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\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

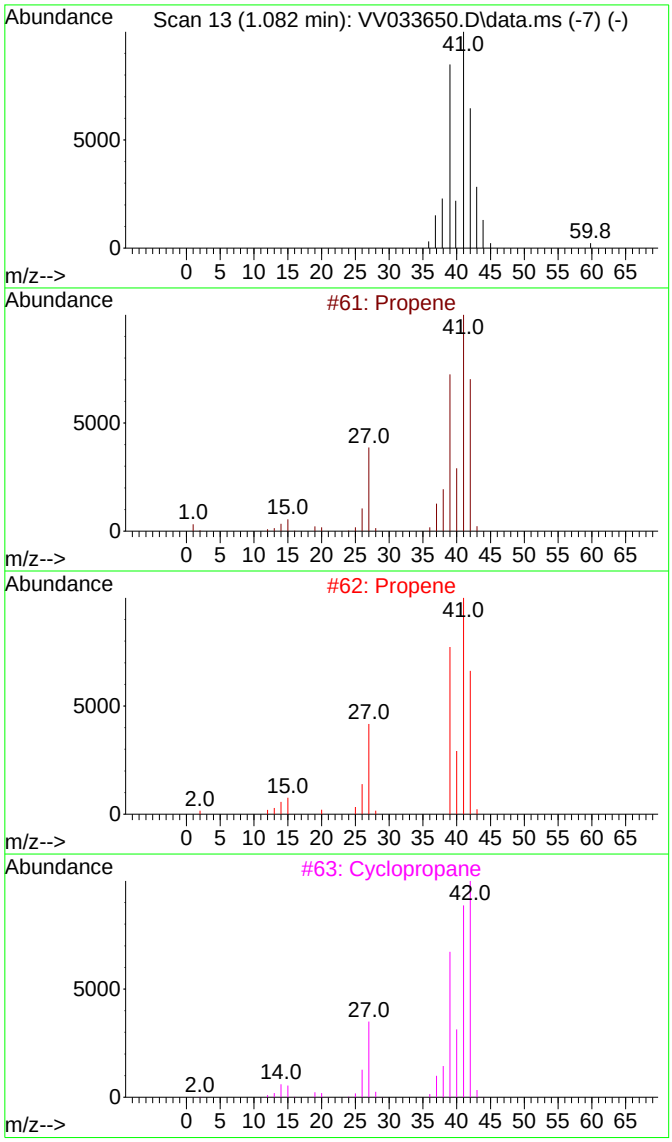
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

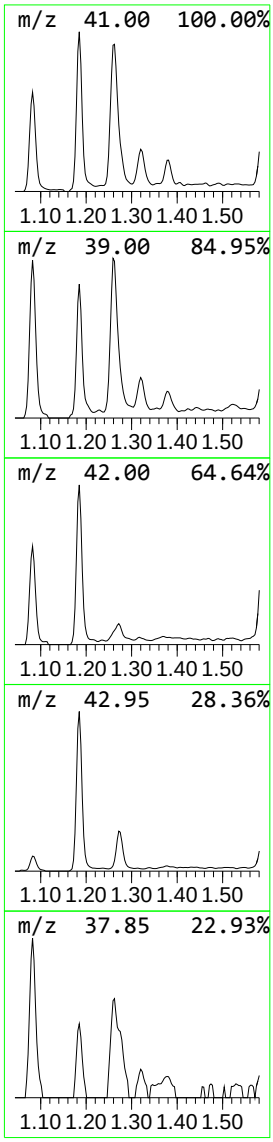
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.082	0.52 ug/L	29884	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propene	42	C3H6	000115-07-1	83
2	Propene	42	C3H6	000115-07-1	45
3	Cyclopropane	42	C3H6	000075-19-4	43
4	Cyclopropane	42	C3H6	000075-19-4	43
5	2-Oxetanone, 4-methyl-	86	C4H6O2	003068-88-0	4





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

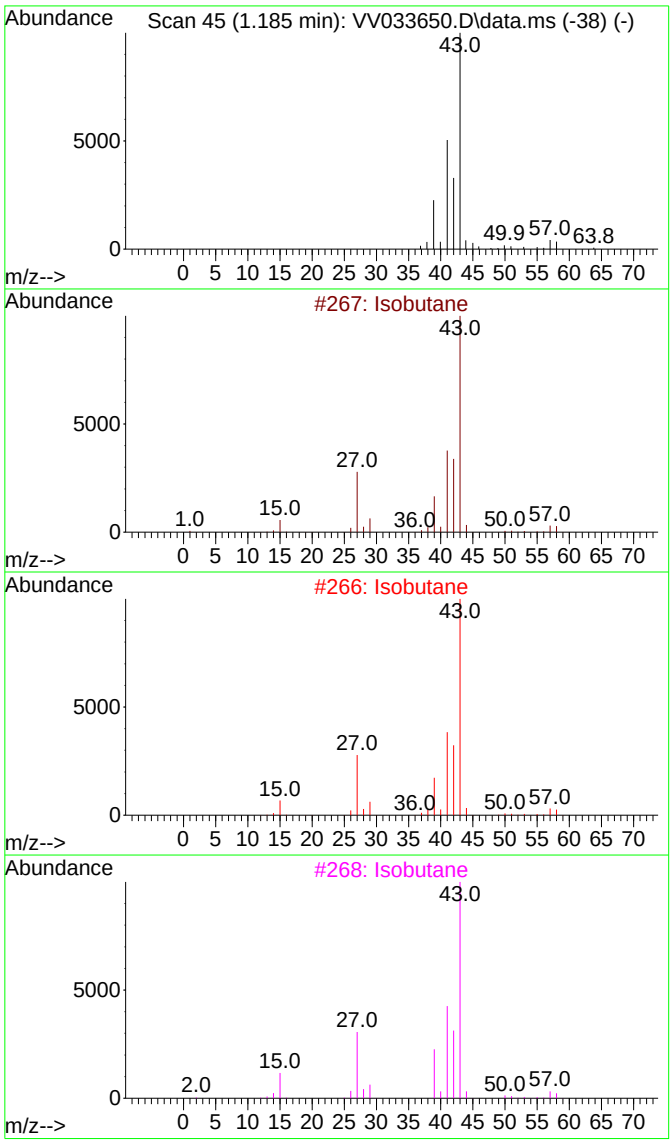
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

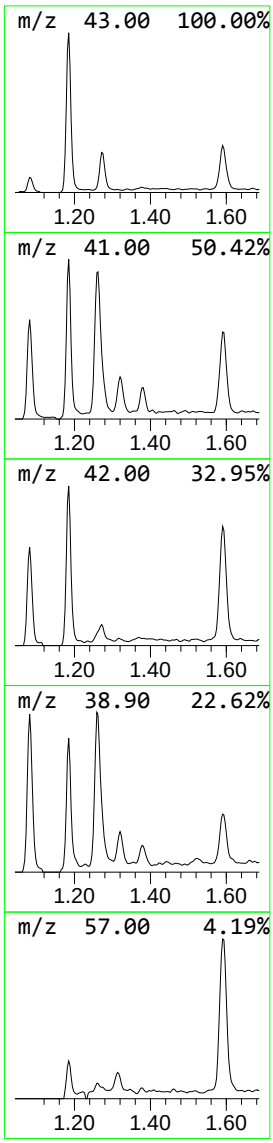
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.185	0.82 ug/L	47030	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isobutane	58	C4H10	000075-28-5	86
2	Isobutane	58	C4H10	000075-28-5	80
3	Isobutane	58	C4H10	000075-28-5	72
4	Isobutane	58	C4H10	000075-28-5	72
5	Isobutane	58	C4H10	000075-28-5	64





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

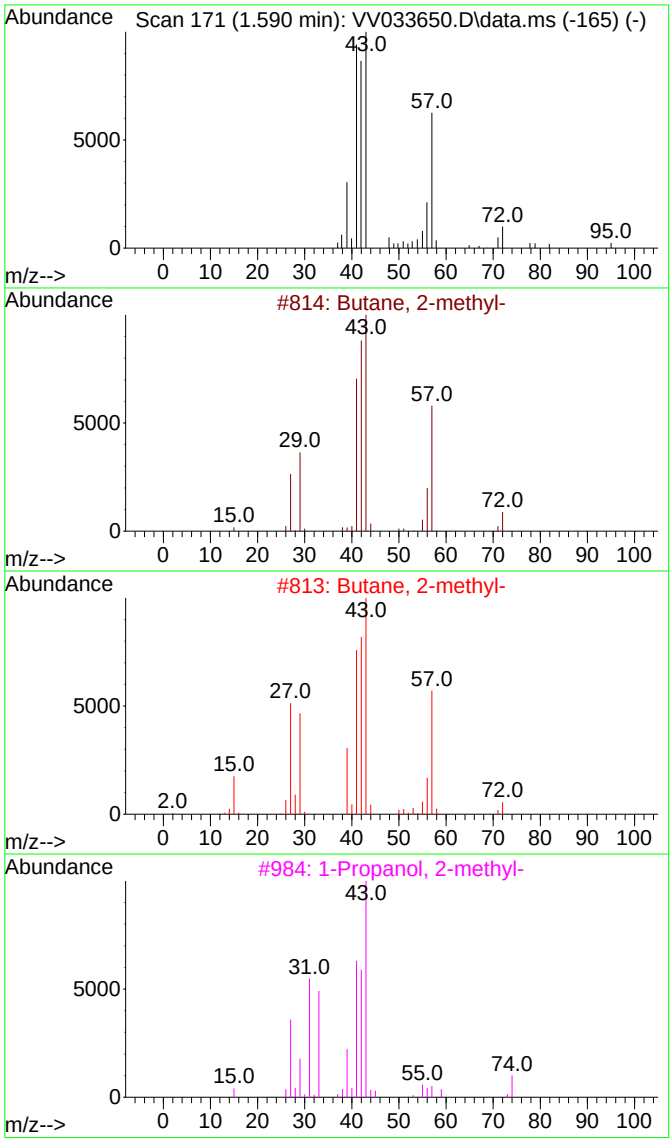
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

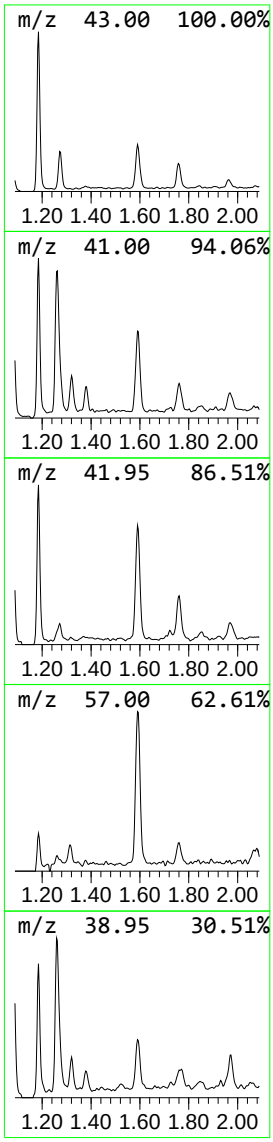
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.590	0.57 ug/L	32654	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-	72	C5H12	000078-78-4	90
2	Butane, 2-methyl-	72	C5H12	000078-78-4	86
3	1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	38
4	Oxirane, trimethyl-	86	C5H10O	005076-19-7	38
5	3-Buten-1-ol	72	C4H8O	000627-27-0	37





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
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Operator : SY/MD
Sample : P1131-18
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ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

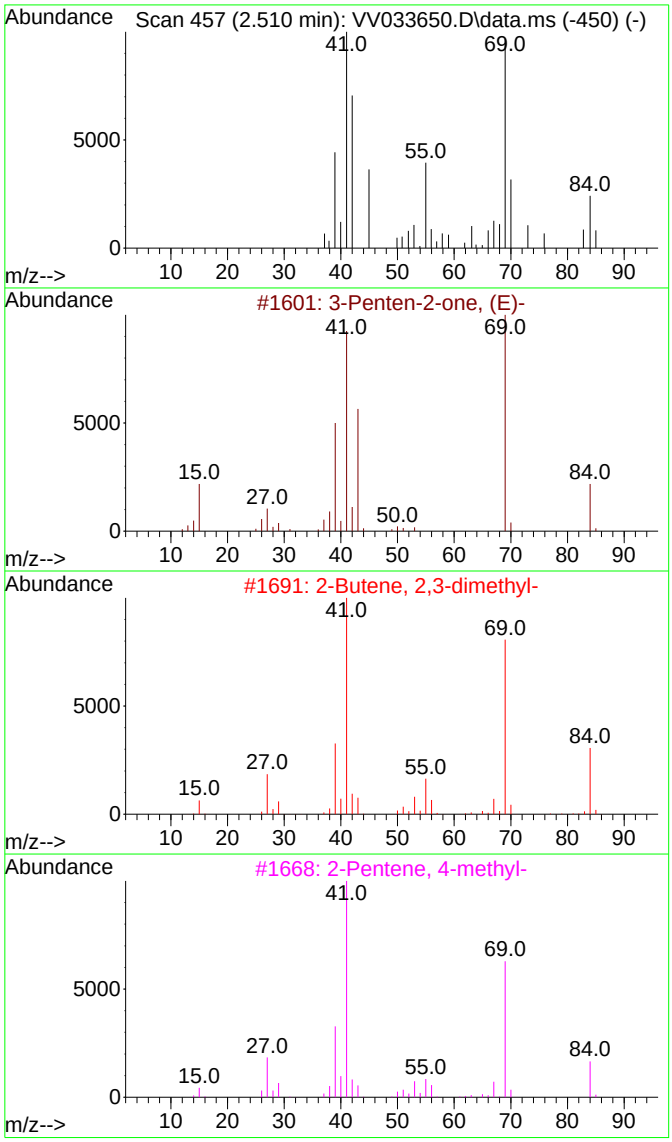
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

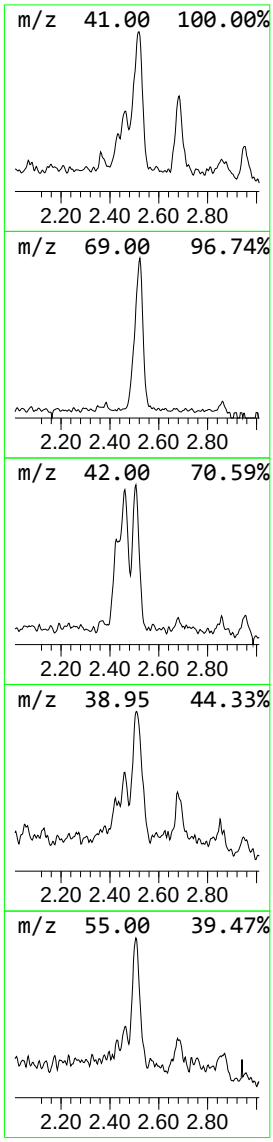
****

Peak Number 4 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.510	0.76 ug/L	43612	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, (E)-	84	C5H8O	003102-33-8	47
2	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	38
3	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	38
4	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	38
5	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	35





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Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

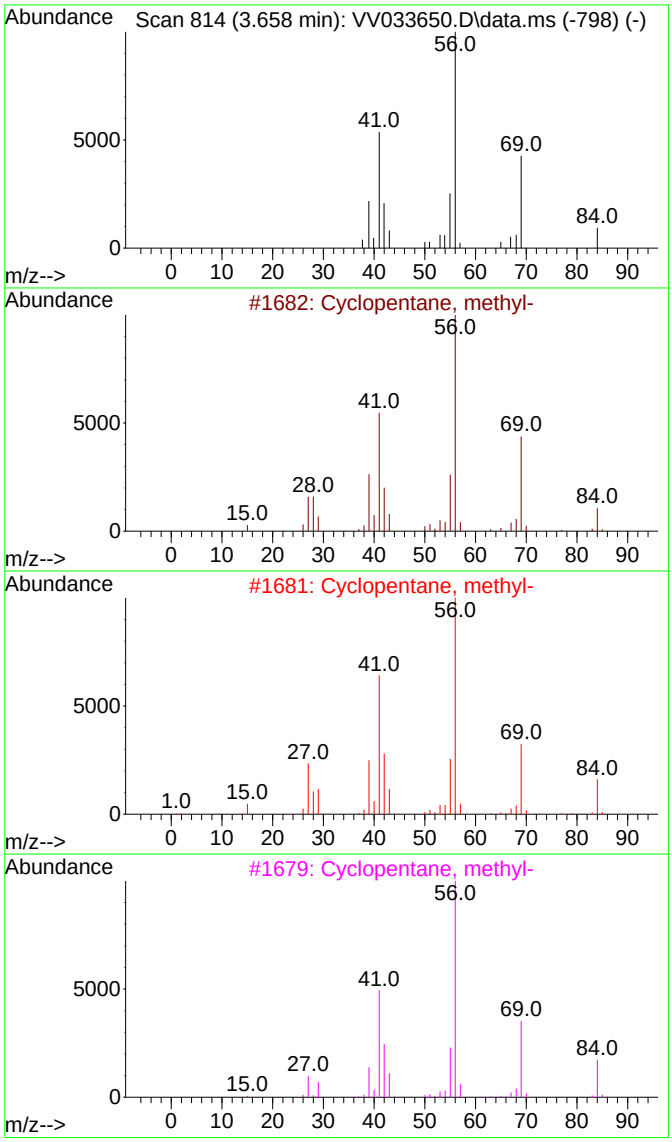
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

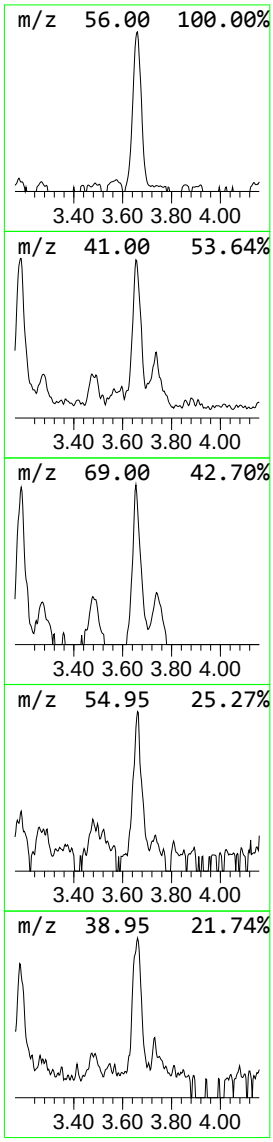
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Cyclic3.658 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.658	0.52 ug/L	29885	1,4-Difluorobenzene	5.532

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2	Cyclopentane, methyl-	84	C6H12	000096-37-7	86
3	Cyclopentane, methyl-	84	C6H12	000096-37-7	80
4	Cyclopentane, methyl-	84	C6H12	000096-37-7	78
5	Cyclobutane, ethyl-	84	C6H12	004806-61-5	72





Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

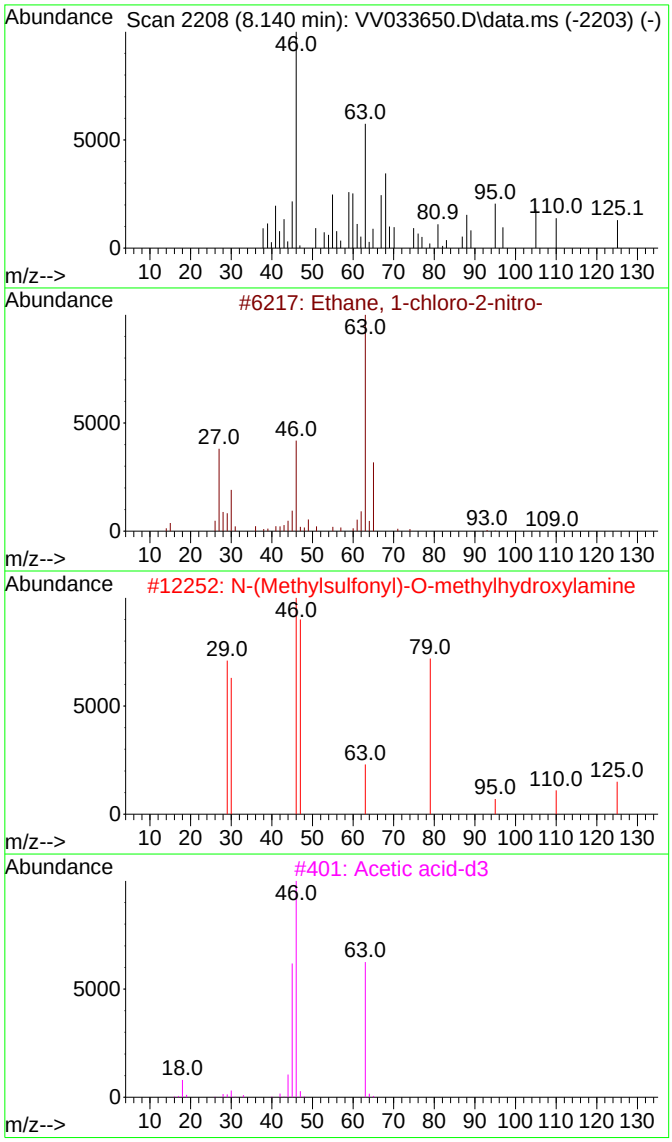
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

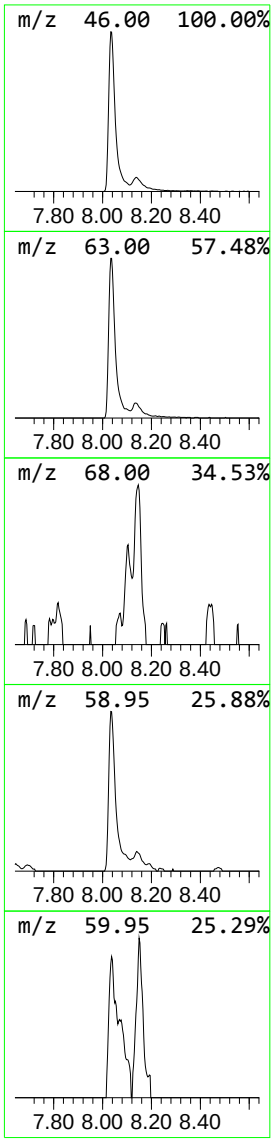
****

Peak Number 7 unknown-02 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.140	0.65 ug/L	41519	Chlorobenzene-d5	8.786

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Ethane, 1-chloro-2-nitro-	109	C2H4ClNO2	000625-47-8	40
2	N-(Methylsulfonyl)-O-methylhydro...	125	C2H7NO3S	080653-53-8	9
3	Acetic acid-d3	63	C2HD3O2	001112-02-3	9
4	Nitroisobutanetriol trinitrate	286	C4H6N4O11	020820-44-4	9
5	1,3-Propanediol, 2-methyl-2-nitr...	225	C4H7N3O8	004055-94-1	9





Tentatively Identified Compound (LSC) summary

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011524\
Data File : VV033650.D
Acq On : 15 Jan 2024 18:09
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
C0AY0

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.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...	1.082	0.5	ug/L	29884	1	5.532	286664	5.0
(DEL) Alkane: S...	1.185	0.8	ug/L	47030	1	5.532	286664	5.0
(DEL) Alkane: S...	1.590	0.6	ug/L	32654	1	5.532	286664	5.0
unknown-01	2.510	0.8	ug/L	43612	1	5.532	286664	5.0
(DEL) Alkane: C...	3.658	0.5	ug/L	29885	1	5.532	286664	5.0
unknown-02	8.140	0.7	ug/L	41519	2	8.786	317901	5.0