

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011624\
 Data File : VV033680.D
 Acq On : 16 Jan 2024 18:56
 Operator : SY/MD
 Sample : P1131-18
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 27 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: VV033680.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	24	rVB2	25051	27454	2.21%	0.410%
2	1.182	38	44	51	rBV	50220	44946	3.62%	0.671%
3	1.275	61	73	82	rBV3	147035	185050	14.89%	2.763%
4	1.526	144	151	162	rVB	35302	41419	3.33%	0.618%
5	1.590	163	171	180	rBV	26463	35939	2.89%	0.537%
6	1.757	216	223	236	rVB3	10770	18297	1.47%	0.273%
7	1.966	283	288	298	rVB3	9572	13071	1.05%	0.195%
8	2.050	305	314	328	rBV	64345	93650	7.53%	1.398%
9	2.458	436	441	447	rVV2	12335	19750	1.59%	0.295%
10	2.506	449	456	475	rVB5	18882	45346	3.65%	0.677%
11	2.680	500	510	522	rBV3	16502	30417	2.45%	0.454%
12	3.101	633	641	652	rVB2	10608	20381	1.64%	0.304%
13	3.175	656	664	673	rBV4	7261	13303	1.07%	0.199%
14	3.645	800	810	825	rVB3	11935	27961	2.25%	0.417%
15	3.802	844	859	875	rBV	235251	556531	44.78%	8.308%
16	4.240	982	995	1015	rVB2	55983	139235	11.20%	2.079%
17	4.558	1085	1094	1108	rVB4	10234	23934	1.93%	0.357%
18	4.944	1201	1214	1224	rBV2	130914	291723	23.47%	4.355%
19	5.214	1290	1298	1313	rVB8	7655	18712	1.51%	0.279%
20	5.526	1380	1395	1428	rBV	124700	268567	21.61%	4.009%
21	5.989	1518	1539	1566	rBV	75697	186382	15.00%	2.782%
22	6.484	1673	1693	1703	rBV7	6624	20501	1.65%	0.306%
23	6.567	1703	1719	1729	rVV7	4719	12464	1.00%	0.186%
24	6.686	1741	1756	1772	rBV10	6860	19879	1.60%	0.297%
25	6.911	1816	1826	1850	rVB	40605	77331	6.22%	1.154%
26	7.088	1867	1881	1893	rVB3	13405	26156	2.10%	0.390%
27	7.239	1915	1928	1944	rVV	147502	264689	21.30%	3.952%
28	7.558	2018	2027	2045	rVB4	25070	55030	4.43%	0.822%
29	8.043	2168	2178	2205	rBV	149356	331032	26.63%	4.942%
30	8.783	2398	2408	2413	rBV	188185	302834	24.36%	4.521%
31	9.040	2471	2488	2490	rBV10	5946	12526	1.01%	0.187%
32	9.075	2491	2499	2511	rVB2	19639	35869	2.89%	0.535%
33	9.198	2524	2537	2544	rBV7	8975	16589	1.33%	0.248%
34	9.403	2586	2601	2603	rBV8	8055	15126	1.22%	0.226%
35	9.635	2665	2673	2691	rVB7	10703	24610	1.98%	0.367%
36	9.738	2691	2705	2716	rBV7	9626	26240	2.11%	0.392%

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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	9.866	2737	2745	2755	rBV	12300	24015	1.93%	0.359%
38	10.056	2797	2804	2814	rVB9	8732	14351	1.15%	0.214%
39	10.156	2825	2835	2851	rVB	53827	90387	7.27%	1.349%
40	10.673	2988	2996	3014	rVB3	23111	52109	4.19%	0.778%
41	10.799	3017	3035	3047	rVB2	15623	35670	2.87%	0.533%
42	10.869	3048	3057	3069	rBV5	14402	27470	2.21%	0.410%
43	10.934	3069	3077	3087	rBV3	13213	21124	1.70%	0.315%
44	10.992	3087	3095	3101	rBV	39338	60382	4.86%	0.901%
45	11.027	3101	3106	3116	rVB	26747	39118	3.15%	0.584%
46	11.117	3125	3134	3144	rBV	90414	140299	11.29%	2.095%
47	11.207	3146	3162	3181	rVB2	617210	1242913	100.00%	18.555%
48	11.394	3210	3220	3230	rVB8	13082	24246	1.95%	0.362%
49	11.574	3256	3276	3300	rVB3	230792	590059	47.47%	8.809%
50	11.686	3303	3311	3321	rBV7	13929	26609	2.14%	0.397%
51	11.779	3335	3340	3353	rVB10	13353	20825	1.68%	0.311%
52	11.921	3377	3384	3394	rBV9	14789	23793	1.91%	0.355%
53	11.992	3399	3406	3417	rVV7	18463	33966	2.73%	0.507%
54	12.062	3419	3428	3444	rVB10	23615	61724	4.97%	0.921%
55	12.130	3445	3449	3457	rVB3	10264	12606	1.01%	0.188%
56	12.181	3457	3465	3472	rBV9	23335	45214	3.64%	0.675%
57	12.233	3476	3481	3489	rVB	25818	38466	3.09%	0.574%
58	12.493	3556	3562	3569	rBV3	11346	15209	1.22%	0.227%
59	12.622	3595	3602	3613	rVB2	39424	59509	4.79%	0.888%
60	12.895	3681	3687	3700	rVB5	12030	20075	1.62%	0.300%
61	13.107	3740	3753	3761	rBV4	15495	36724	2.95%	0.548%
62	13.204	3776	3783	3789	rBV4	22982	38263	3.08%	0.571%
63	13.249	3790	3797	3801	rBV2	26780	42004	3.38%	0.627%
64	13.484	3864	3870	3878	rVB6	17741	26182	2.11%	0.391%
65	13.545	3881	3889	3902	rVB5	31545	60383	4.86%	0.901%
66	13.635	3903	3917	3937	rBV5	27479	96167	7.74%	1.436%
67	13.776	3952	3961	3970	rVB5	9090	20223	1.63%	0.302%
68	14.046	4035	4045	4056	rVB7	11445	25362	2.04%	0.379%
69	14.168	4075	4083	4094	rVV	33068	49652	3.99%	0.741%
70	14.236	4097	4104	4113	rVB4	20379	31157	2.51%	0.465%
71	14.381	4139	4149	4160	rBV5	17494	36276	2.92%	0.542%
72	14.619	4214	4223	4239	rVB5	13638	35905	2.89%	0.536%
73	14.766	4259	4269	4280	rVB5	19116	42023	3.38%	0.627%
74	14.956	4322	4328	4340	rVB3	13302	20504	1.65%	0.306%
75	15.104	4362	4374	4384	rBV2	14659	26314	2.12%	0.393%
76	15.268	4415	4425	4436	rVB9	10585	25508	2.05%	0.381%

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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

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Peak separation: 5

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

77	15.381	4449	4460	4472	rVB7	8856	22679	1.82%	0.339%
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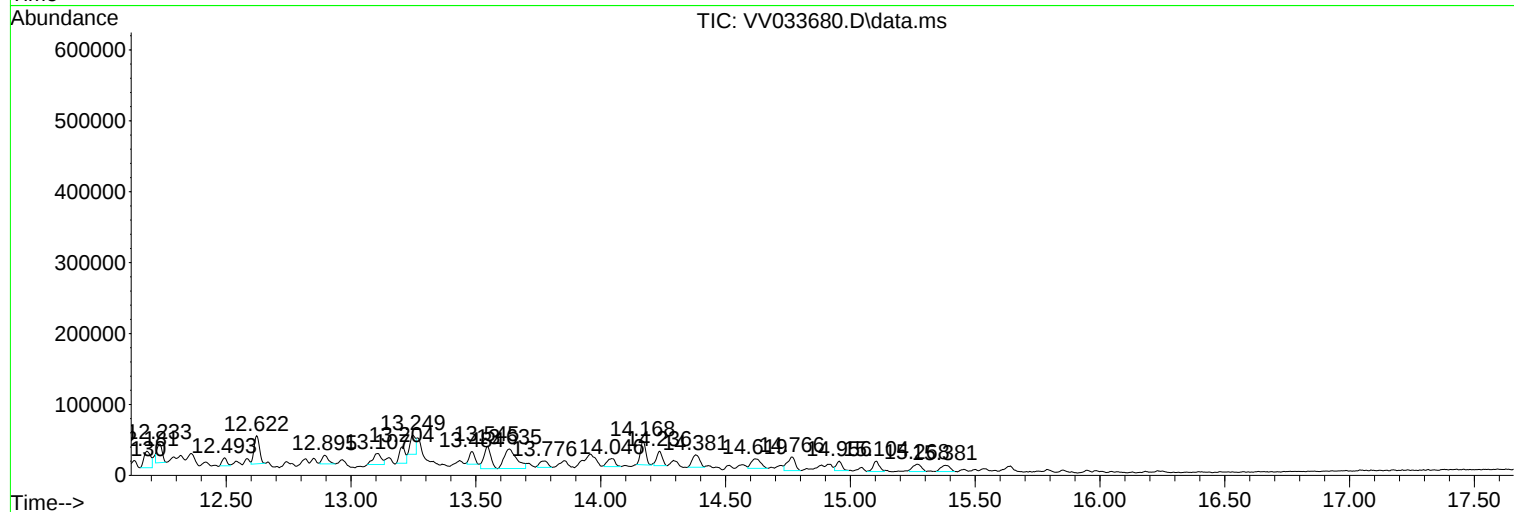
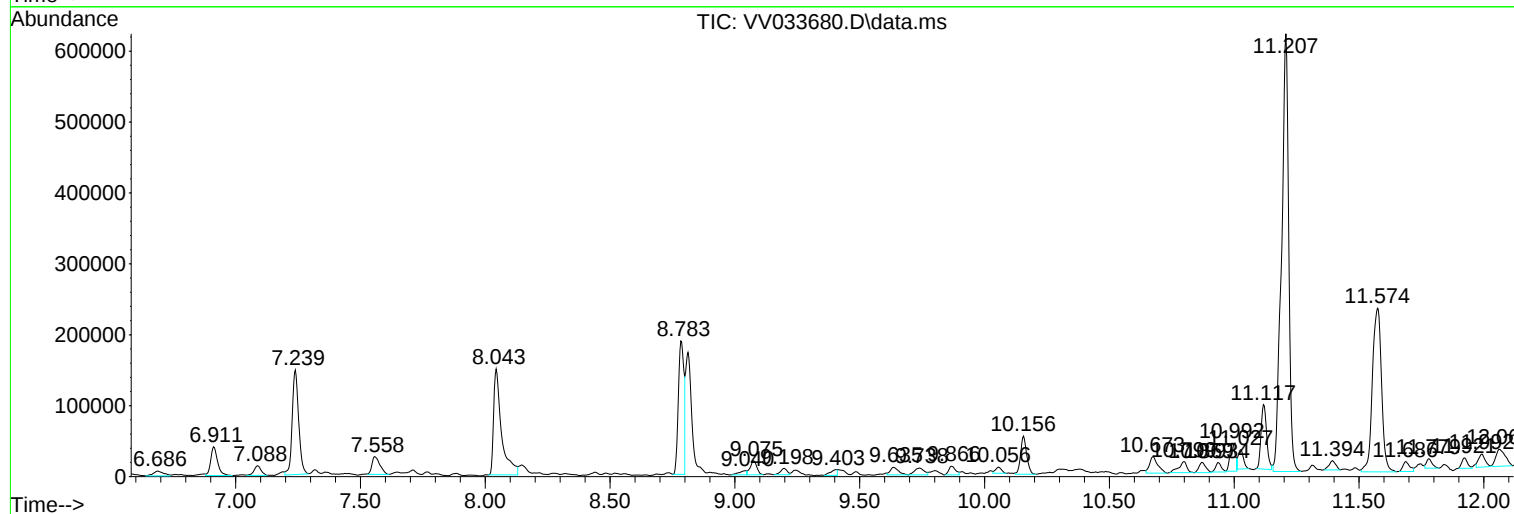
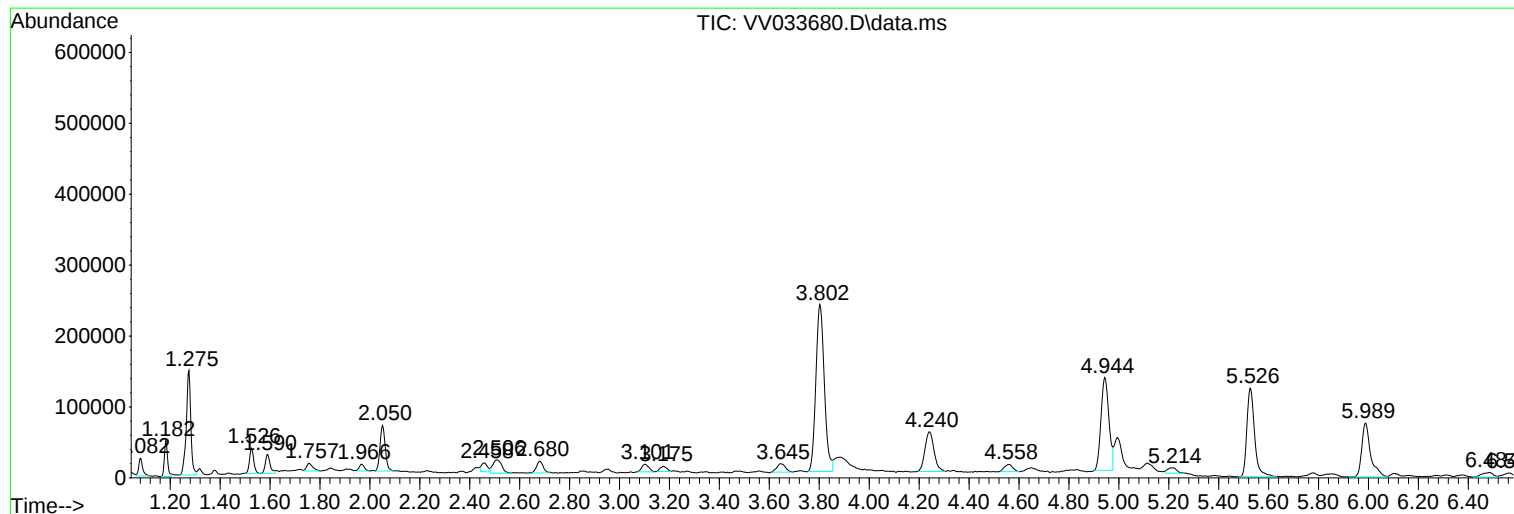
Sum of corrected areas: 6698409

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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



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Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
COAY0

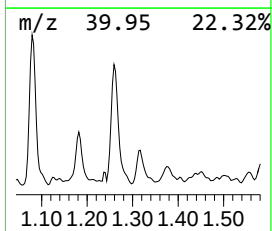
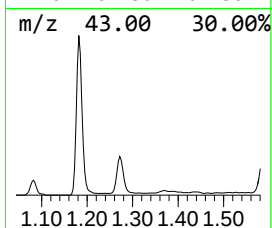
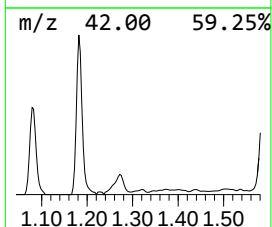
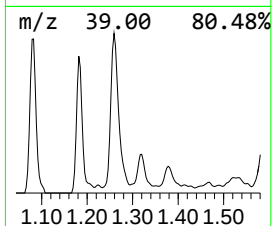
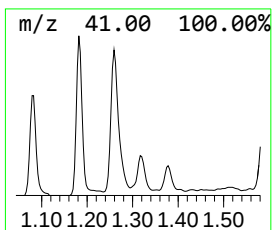
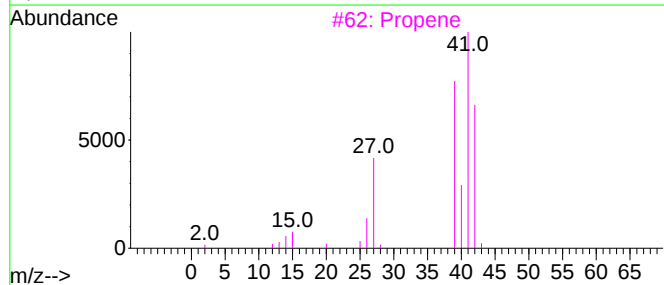
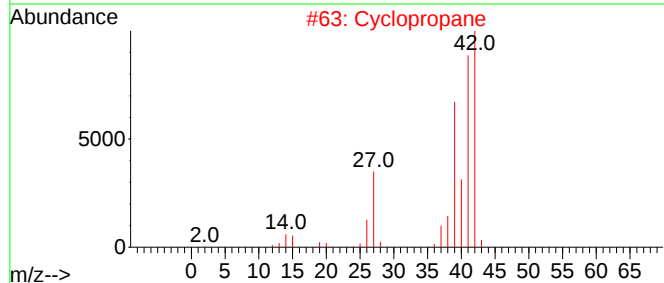
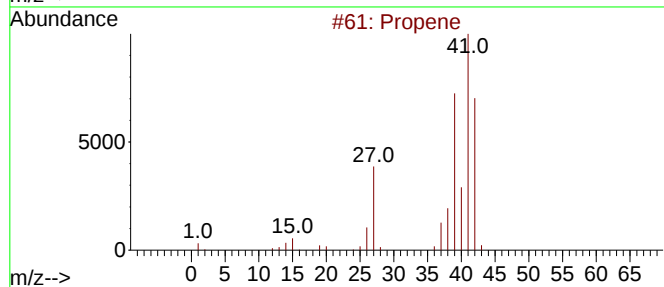
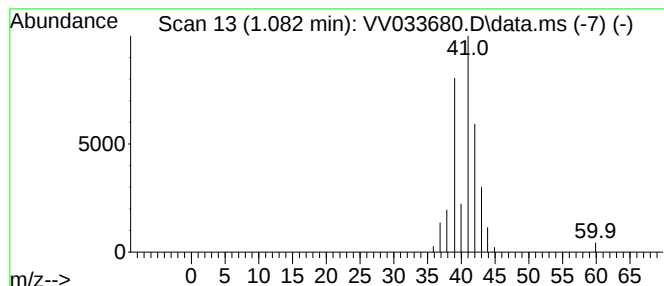
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.082	0.51 ug/L	27454	1,4-Difluorobenzene	5.526

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	43
3			Propene	42	C3H6	000115-07-1	42
4			Cyclopropene	40	C3H4	002781-85-3	9
5			Cyclopropane	42	C3H6	000075-19-4	7



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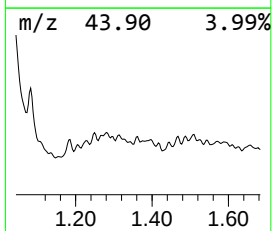
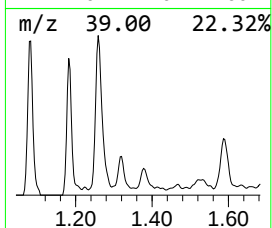
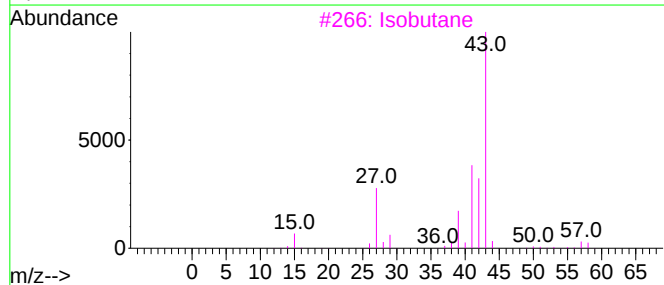
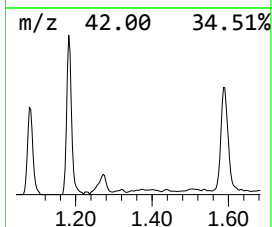
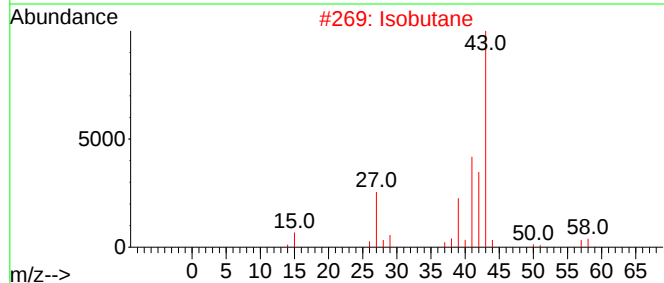
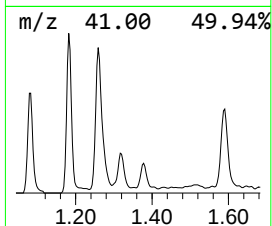
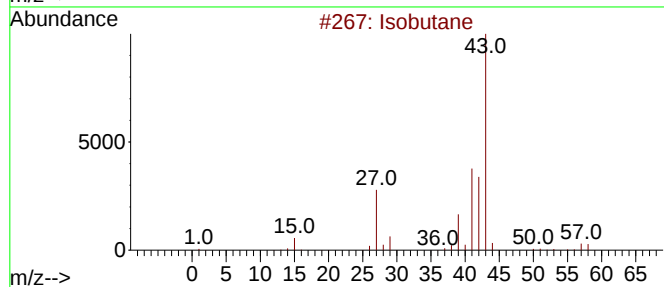
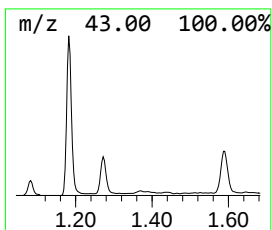
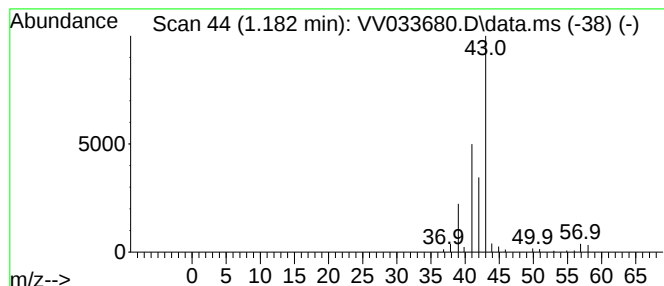
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 (DEL) Alkane: Straight-Chai... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.182	0.84 ug/L	44946	1,4-Difluorobenzene	5.526

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Isobutane	58	C4H10	000075-28-5	80
2		Isobutane	58	C4H10	000075-28-5	72
3		Isobutane	58	C4H10	000075-28-5	72
4		Isobutane	58	C4H10	000075-28-5	64
5		Isobutane	58	C4H10	000075-28-5	59



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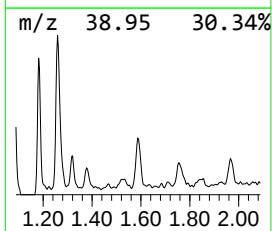
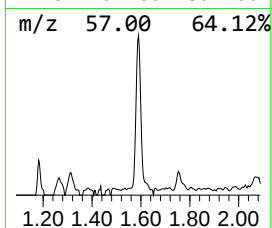
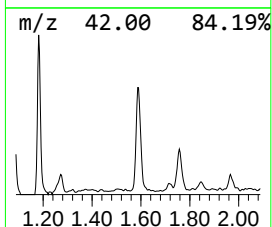
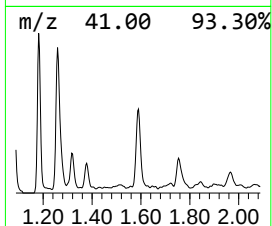
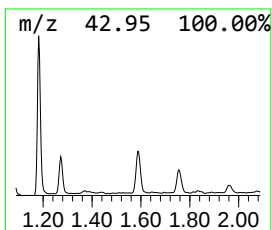
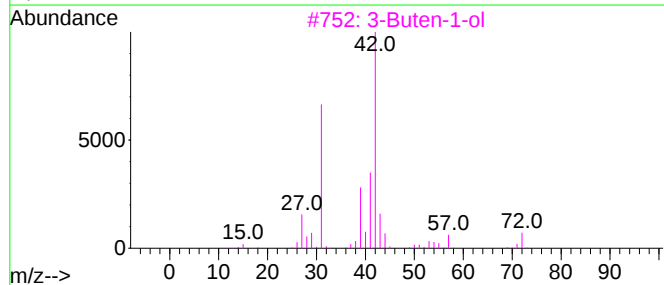
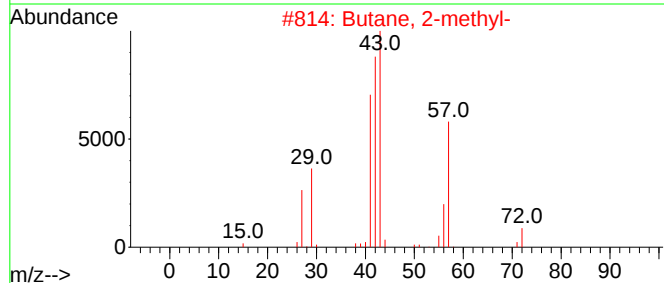
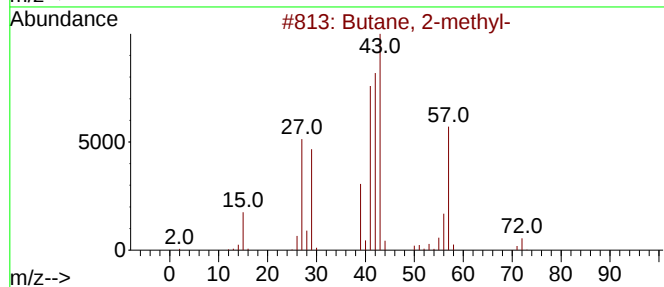
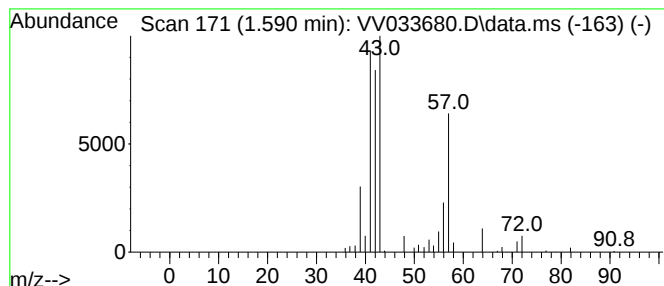
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR011224WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.590	0.67 ug/L	35939	1,4-Difluorobenzene	5.526

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methyl-	72	C5H12	000078-78-4	86
2		Butane, 2-methyl-	72	C5H12	000078-78-4	72
3		3-Buten-1-ol	72	C4H8O	000627-27-0	43
4		Oxirane, trimethyl-	86	C5H10O	005076-19-7	36
5		Butane, 1-isocyano-	83	C5H9N	002769-64-4	10



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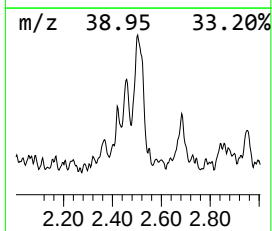
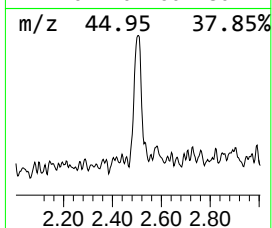
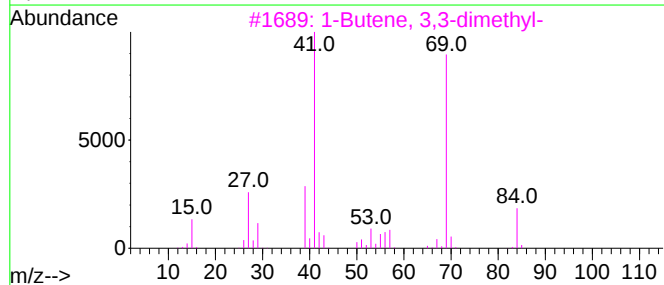
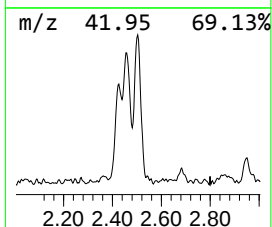
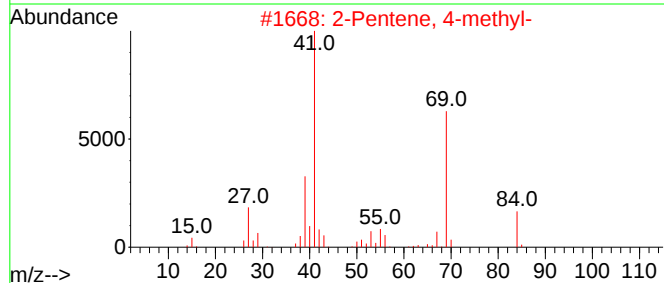
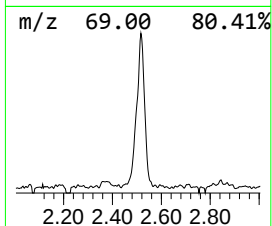
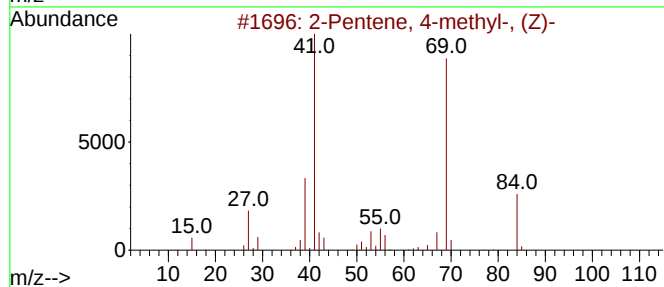
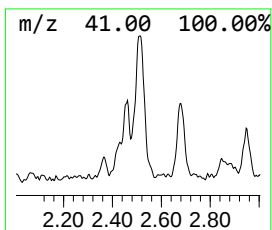
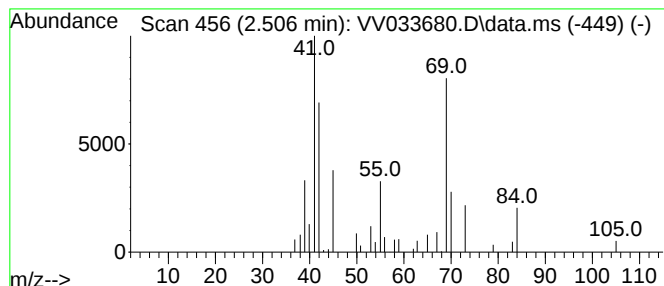
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.506	0.84 ug/L	45346	1,4-Difluorobenzene	5.526

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, 4-methyl-, (Z)-	84	C6H12	000691-38-3	49	
2	2-Pentene, 4-methyl-	84	C6H12	004461-48-7	49	
3	1-Butene, 3,3-dimethyl-	84	C6H12	000558-37-2	47	
4	2-Butene, 2,3-dimethyl-	84	C6H12	000563-79-1	47	
5	Acetaldehyde, ethylidenehydrazone	84	C4H8N2	000592-56-3	47	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011624\
Data File : VV033680.D
Acq On : 16 Jan 2024 18:56
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 27 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
COAY0

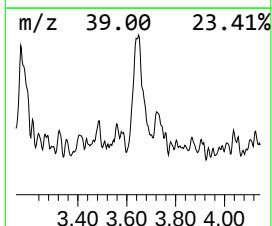
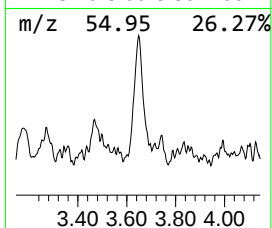
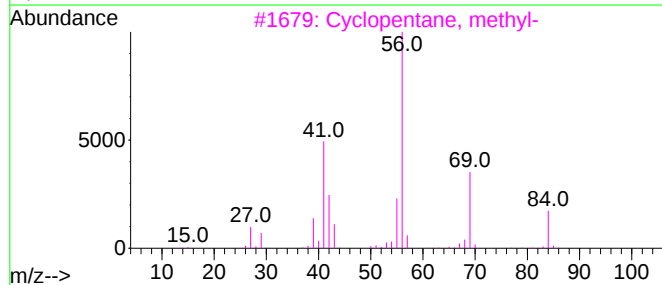
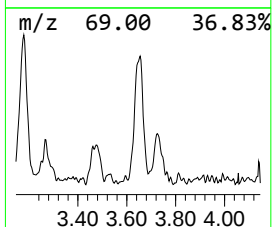
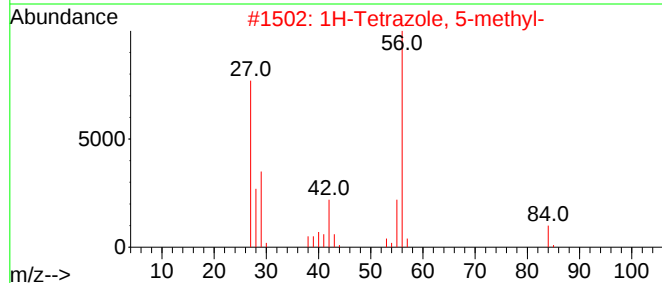
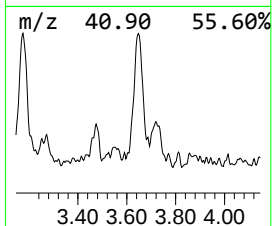
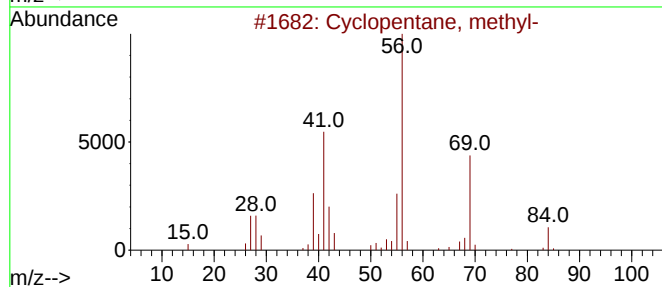
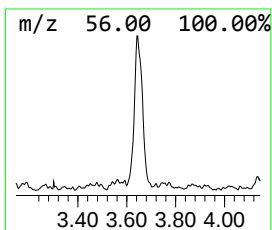
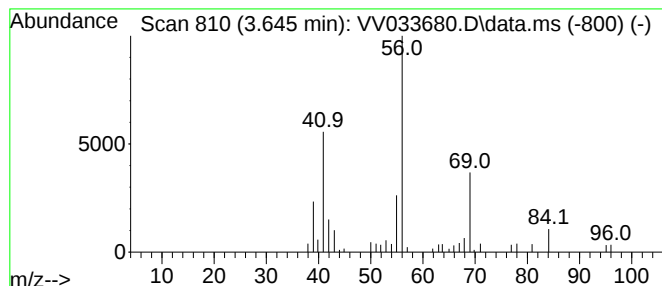
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Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 (DEL) Alkane: Cyclic3.645 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.645	0.52 ug/L	27961	1,4-Difluorobenzene	5.526

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Cyclopentane, methyl-	84	C6H12	000096-37-7	81
2		1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3		Cyclopentane, methyl-	84	C6H12	000096-37-7	53
4		Cyclopentane, methyl-	84	C6H12	000096-37-7	53
5		1-Hexene, 5-methyl-	98	C7H14	003524-73-0	45



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011624\
Data File : VV033680.D
Acq On : 16 Jan 2024 18:56
Operator : SY/MD
Sample : P1131-18
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 27 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	27454	1	5.526	268567	5.0
(DEL)	Alkane: S...	1.182	0.8	ug/L	44946	1	5.526	268567	5.0
(DEL)	Alkane: S...	1.590	0.7	ug/L	35939	1	5.526	268567	5.0
(DEL)	Alkane: S...	2.506	0.8	ug/L	45346	1	5.526	268567	5.0
(DEL)	Alkane: C...	3.645	0.5	ug/L	27961	1	5.526	268567	5.0