

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV121323\
 Data File : VV033296.D
 Acq On : 13 Dec 2023 23:08
 Operator : SY/MD
 Sample : 05731-22
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 EOY68

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\SFAMVTR121323WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV033296.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.085	8	14	29	rVB	500227	467135	100.00%	8.449%
2	1.191	41	47	53	rBV	61122	54479	11.66%	0.985%
3	1.275	63	73	85	rBV3	215489	326721	69.94%	5.910%
4	1.388	102	108	115	rVB	16455	18445	3.95%	0.334%
5	1.532	145	153	164	rVB	53813	66800	14.30%	1.208%
6	1.597	164	173	186	rVB	32245	42080	9.01%	0.761%
7	1.671	187	196	205	rVB	13569	17135	3.67%	0.310%
8	1.728	205	214	220	rBV	31098	40043	8.57%	0.724%
9	1.770	220	227	244	rVB3	38932	67392	14.43%	1.219%
10	1.857	249	254	264	rVB3	3565	5218	1.12%	0.094%
11	1.937	268	279	287	rBV4	10981	16140	3.46%	0.292%
12	2.060	307	317	329	rBV	99072	146737	31.41%	2.654%
13	2.388	405	419	431	rBV7	6453	15700	3.36%	0.284%
14	2.471	439	445	453	rVB4	6976	10373	2.22%	0.188%
15	2.696	502	515	527	rBV5	8295	15918	3.41%	0.288%
16	2.883	557	573	585	rVB2	11117	24843	5.32%	0.449%
17	2.969	588	600	616	rVB3	9603	19035	4.07%	0.344%
18	3.378	714	727	737	rBV8	2901	6216	1.33%	0.112%
19	3.815	849	863	905	rBV2	130969	375354	80.35%	6.789%
20	4.249	981	998	1024	rBV	80650	227693	48.74%	4.118%
21	4.580	1091	1101	1112	rVB6	4087	8806	1.89%	0.159%
22	4.822	1163	1176	1188	rBV7	2739	6569	1.41%	0.119%
23	4.957	1203	1218	1252	rBV3	167209	453506	97.08%	8.203%
24	5.413	1350	1360	1371	rBV7	3314	6892	1.48%	0.125%
25	5.535	1387	1398	1425	rBV	128801	272741	58.39%	4.933%
26	5.838	1482	1492	1513	rVB2	34140	73519	15.74%	1.330%
27	5.989	1526	1539	1556	rBV2	88333	191431	40.98%	3.463%
28	6.326	1635	1644	1653	rBV6	2661	5454	1.17%	0.099%
29	6.915	1813	1827	1849	rBV	43535	85242	18.25%	1.542%
30	7.243	1918	1929	1943	rBV	213720	382467	81.88%	6.918%
31	7.317	1943	1952	1973	rVB	98573	177230	37.94%	3.206%
32	7.558	2017	2027	2050	rBV3	26922	54181	11.60%	0.980%
33	7.911	2130	2137	2145	rVB5	2999	4912	1.05%	0.089%
34	8.027	2163	2173	2206	rBV	143973	292193	62.55%	5.285%
35	8.786	2394	2409	2437	rBV	200029	353754	75.73%	6.399%
36	8.950	2449	2460	2474	rBV	69948	113934	24.39%	2.061%

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Stop Thrs : 0

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If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	9.075	2490	2499	2511	rBV3	22555	38058	8.15%	0.688%
38	9.500	2615	2631	2650	rBV2	48052	101260	21.68%	1.832%
39	9.873	2738	2747	2758	rVB2	6956	10537	2.26%	0.191%
40	10.156	2824	2835	2852	rBV2	63043	101787	21.79%	1.841%
41	10.294	2868	2878	2886	rBV3	5048	8355	1.79%	0.151%
42	10.390	2897	2908	2925	rBV4	7696	17005	3.64%	0.308%
43	10.480	2925	2936	2944	rVB3	4543	7489	1.60%	0.135%
44	10.677	2990	2997	3006	rBV2	3378	5129	1.10%	0.093%
45	10.857	3041	3053	3067	rBV2	17538	27148	5.81%	0.491%
46	11.188	3145	3156	3176	rBV	203520	327037	70.01%	5.915%
47	11.275	3176	3183	3194	rVB2	7112	10611	2.27%	0.192%
48	11.561	3261	3272	3294	rVB	202917	336977	72.14%	6.095%
49	11.959	3384	3396	3402	rBV3	5057	7512	1.61%	0.136%
50	12.352	3511	3518	3527	rVV2	4472	6058	1.30%	0.110%
51	12.406	3527	3535	3545	rVB3	7225	11055	2.37%	0.200%
52	12.821	3656	3664	3677	rVB4	7904	11923	2.55%	0.216%
53	13.210	3777	3785	3791	rBV7	5859	8044	1.72%	0.145%
54	13.448	3846	3859	3868	rBV3	5419	8359	1.79%	0.151%
55	14.046	4032	4045	4052	rBV7	2974	5438	1.16%	0.098%
56	14.577	4200	4210	4218	rBV3	4977	7818	1.67%	0.141%
57	14.760	4257	4267	4279	rVB7	4059	6991	1.50%	0.126%
58	16.252	4722	4731	4738	rBV	12545	17784	3.81%	0.322%

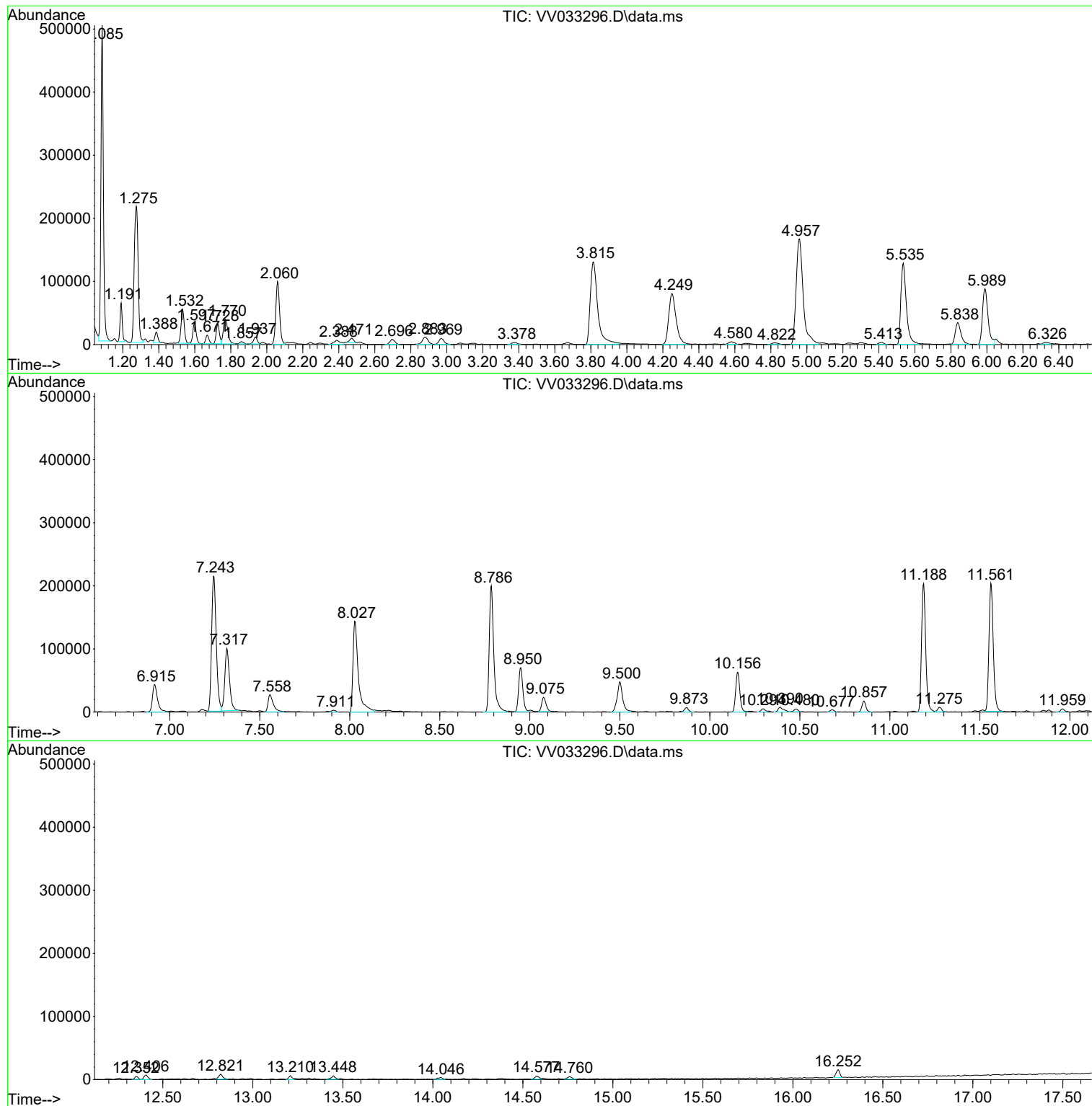
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Quant Title : TRACE VOA SFAM1.0

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



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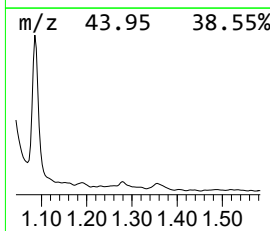
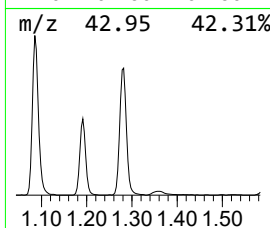
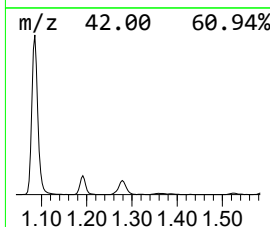
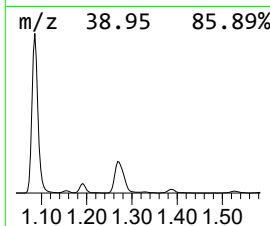
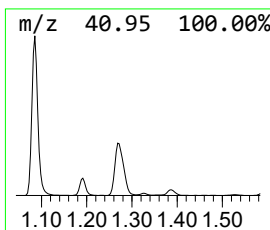
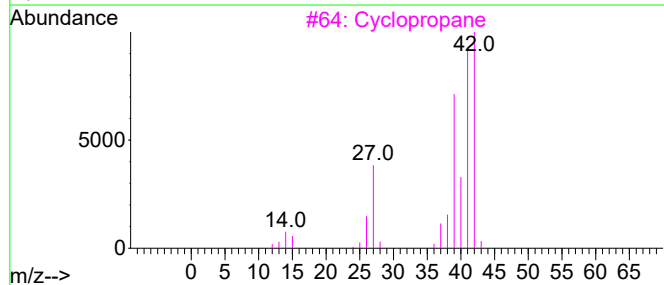
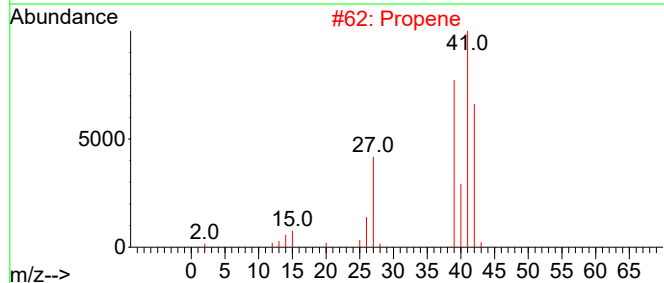
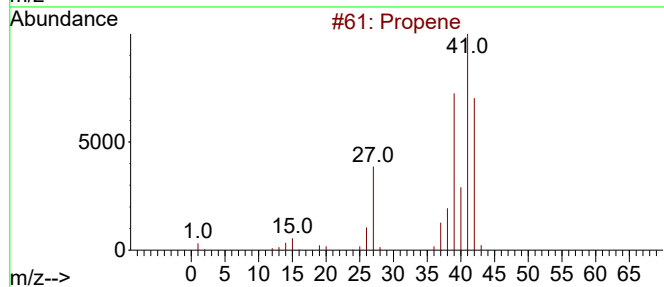
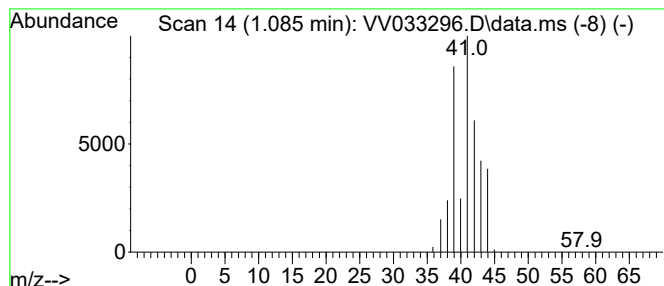
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Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.085	8.56 ug/L	467135	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			Propene	42	C3H6	000115-07-1	40
3			Cyclopropane	42	C3H6	000075-19-4	9
4			Cyclopropane	42	C3H6	000075-19-4	7
5			Cyclopropene	40	C3H4	002781-85-3	5



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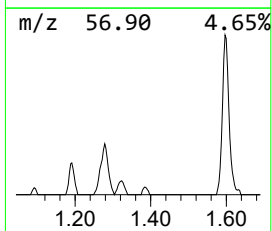
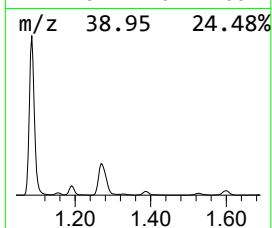
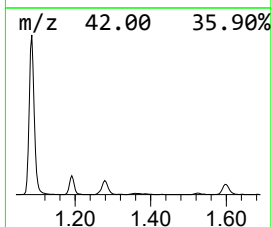
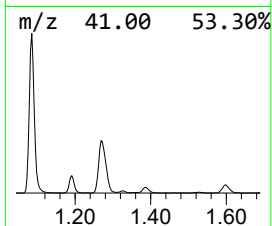
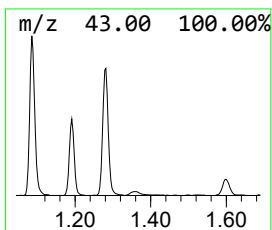
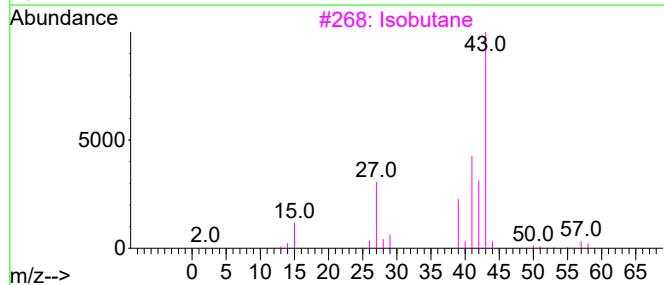
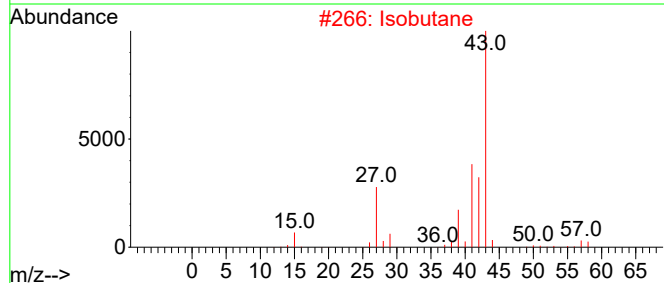
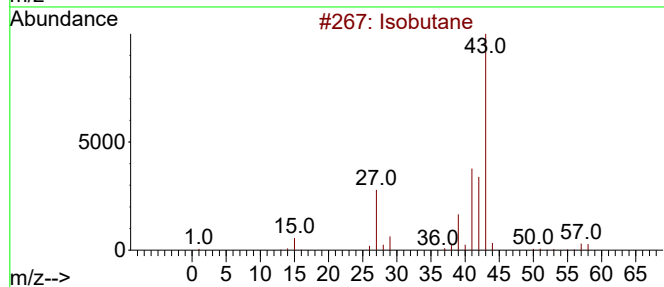
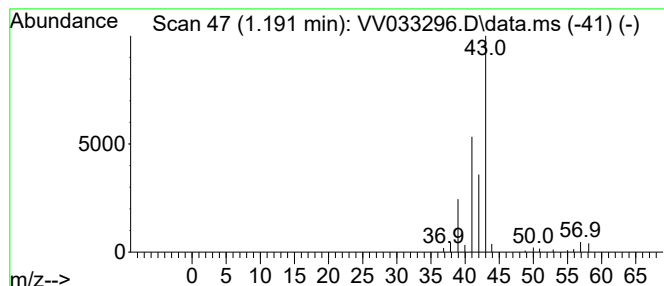
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.191	1.00 ug/L	54479	1,4-Difluorobenzene	5.535

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



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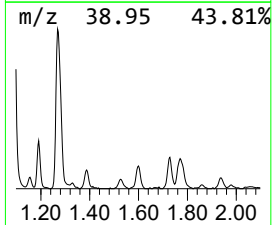
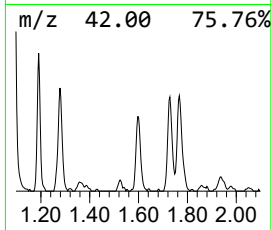
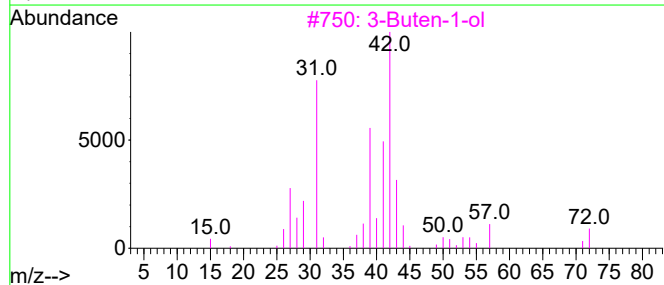
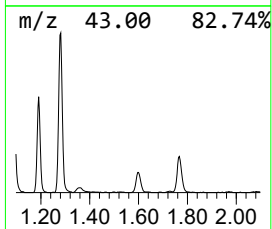
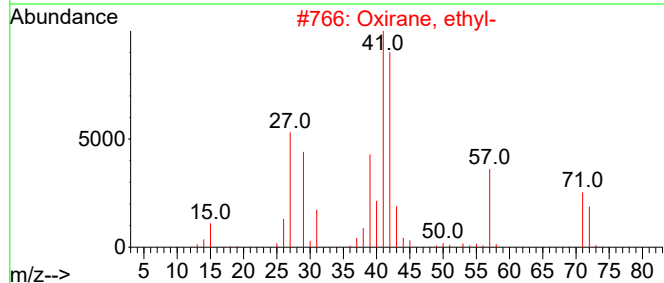
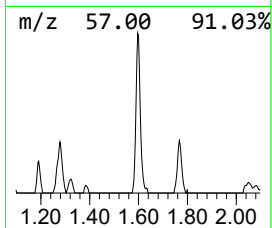
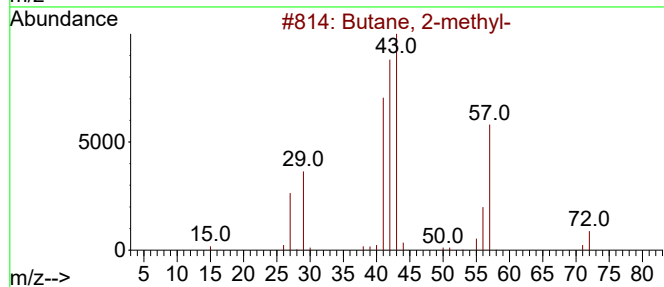
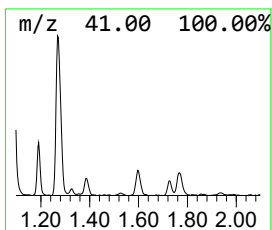
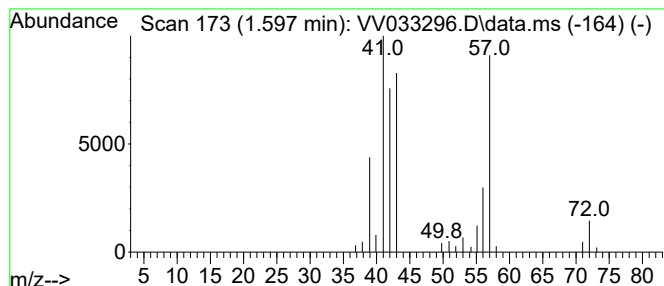
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121323WMA.M
Quant Title : TRACE VOA SFAM1.0

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.
1.597	0.77 ug/L	42080	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methyl-			72	C5H12	000078-78-4	59
2	Oxirane, ethyl-			72	C4H8O	000106-88-7	42
3	3-Buten-1-ol			72	C4H8O	000627-27-0	33
4	2-Methylene-1,3-propanediol			88	C4H8O2	003513-81-3	33
5	1-Propene, 2-methyl-			56	C4H8	000115-11-7	30



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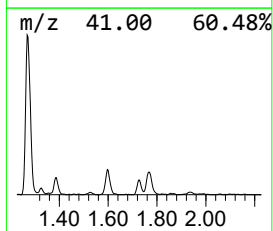
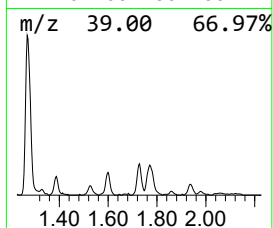
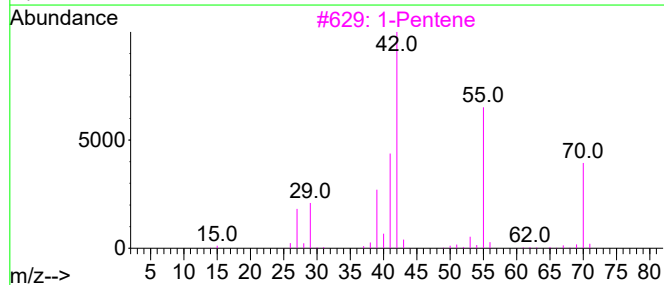
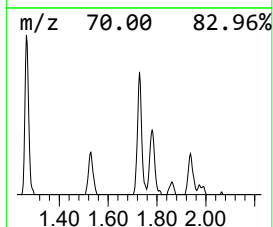
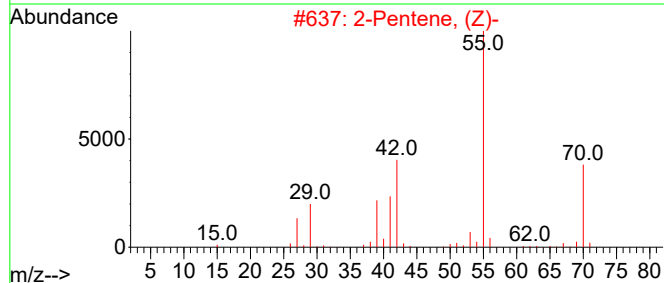
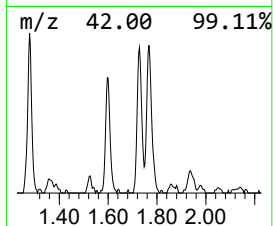
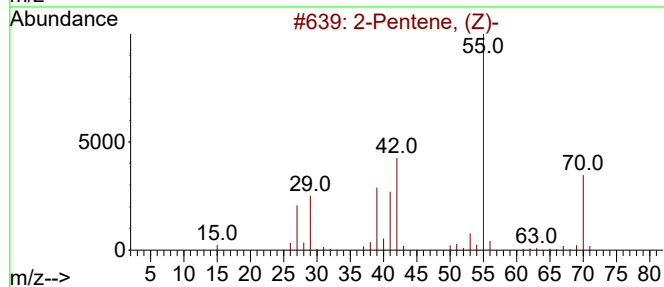
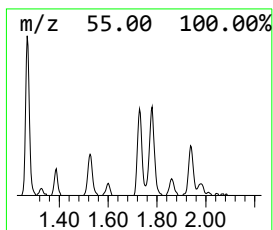
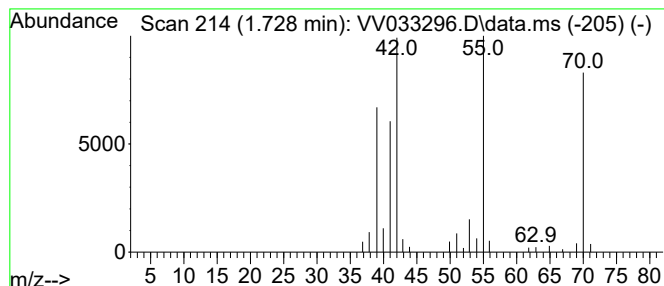
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.728	0.73 ug/L	40043	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentene, (Z)-			70	C5H10	000627-20-3	86
2	2-Pentene, (Z)-			70	C5H10	000627-20-3	86
3	1-Pentene			70	C5H10	000109-67-1	72
4	2-Pentene			70	C5H10	000109-68-2	72
5	Cyclopropane, ethyl-			70	C5H10	001191-96-4	72



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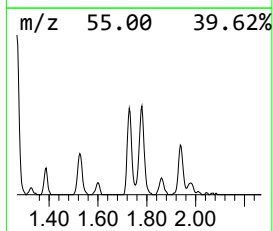
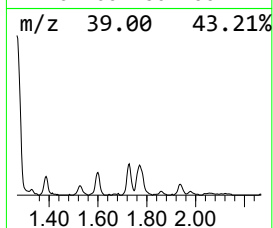
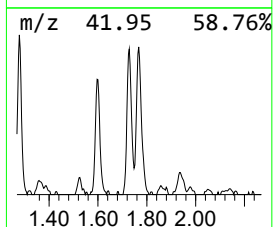
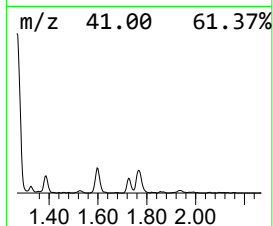
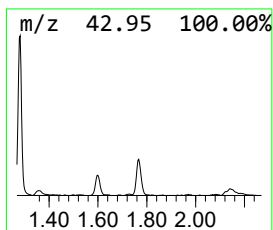
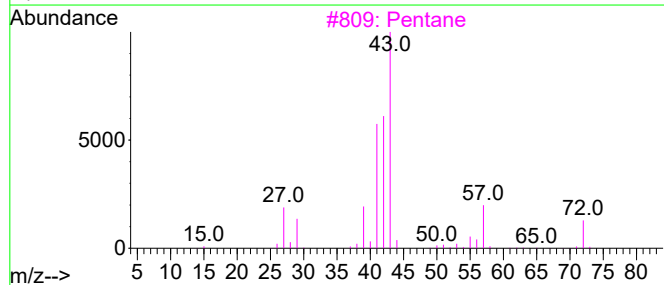
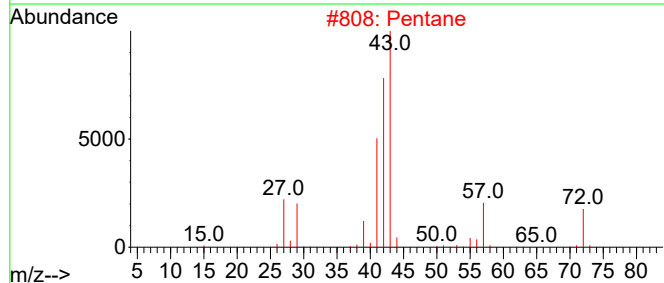
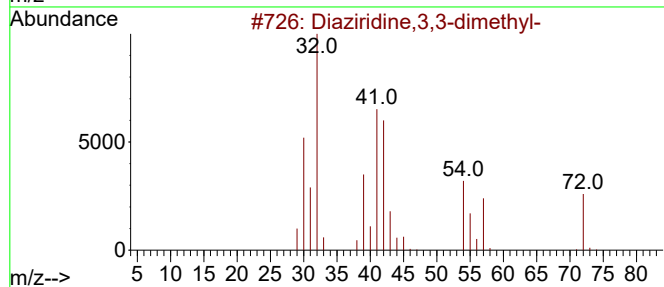
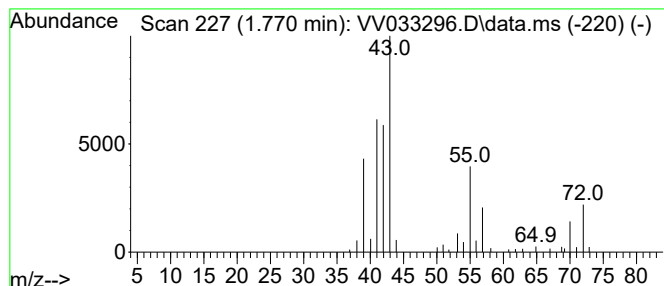
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121323WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 Diaziridine,3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.770	1.24 ug/L	67392	1,4-Difluorobenzene	5.535

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	52
2			Pentane	72	C5H12	000109-66-0	43
3			Pentane	72	C5H12	000109-66-0	43
4			Pentane	72	C5H12	000109-66-0	43
5			Diaziridine,3,3-dimethyl-	72	C3H8N2	004901-76-2	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VW121323\
Data File : VV033296.D
Acq On : 13 Dec 2023 23:08
Operator : SY/MD
Sample : 05731-22
Misc : 25.0mL/MSVOA_V/WATER
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
E0Y68

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR121323WMA.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
(DEL) Alkane: S...	1.085	8.6	ug/L	467135	1	5.535	272741	5.0
(DEL) Alkane: S...	1.191	1.0	ug/L	54479	1	5.535	272741	5.0
(DEL) Alkane: S...	1.597	0.8	ug/L	42080	1	5.535	272741	5.0
(DEL) Alkane: S...	1.728	0.7	ug/L	40043	1	5.535	272741	5.0
Diaziridine,3,3...	1.770	1.2	ug/L	67392	1	5.535	272741	5.0