

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV062322\
 Data File : VV026526.D
 Acq On : 23 Jun 2022 19:55
 Operator : SY/MD
 Sample : N3400-19
 Misc : 25.0mL/MSVOA_V/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 C0AF4

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\SFAMVTR062322WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VV026526.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.269	54	71	72	rBV2	14178	25457	2.57%	0.308%
2	1.317	78	86	107	rVB	138826	165555	16.69%	2.002%
3	1.577	160	167	176	rBV	106846	124987	12.60%	1.512%
4	2.117	326	335	351	rVB	223811	318207	32.08%	3.849%
5	2.223	351	368	399	rBV2	15191	72065	7.26%	0.872%
6	2.748	500	531	532	rBV3	29322	99099	9.99%	1.199%
7	3.696	807	826	855	rBV	356464	973557	98.13%	11.775%
8	3.928	887	898	932	rBV	40184	185451	18.69%	2.243%
9	4.358	1015	1032	1060	rBV	127202	317097	31.96%	3.835%
10	4.686	1118	1134	1150	rVB5	7974	19584	1.97%	0.237%
11	5.053	1233	1248	1282	rBV2	293116	725490	73.13%	8.775%
12	5.622	1408	1425	1451	rBV	255277	517764	52.19%	6.263%
13	6.075	1553	1566	1602	rBV	158815	334320	33.70%	4.044%
14	6.538	1689	1710	1720	rBV	473046	992064	100.00%	11.999%
15	6.992	1839	1851	1869	rBV2	50558	97259	9.80%	1.176%
16	7.317	1940	1952	1977	rBV	357163	633614	63.87%	7.664%
17	7.628	2040	2049	2074	rBV2	24476	47928	4.83%	0.580%
18	7.940	2135	2146	2156	rBV4	7143	12529	1.26%	0.152%
19	8.095	2184	2194	2234	rBV2	227112	495413	49.94%	5.992%
20	8.853	2415	2430	2452	rBV	376979	611449	61.63%	7.396%
21	10.217	2843	2854	2872	rBV	107274	171082	17.25%	2.069%
22	10.381	2890	2905	2915	rVB4	6442	12817	1.29%	0.155%
23	10.776	3018	3028	3042	rBV	9351	14759	1.49%	0.179%
24	11.249	3163	3175	3196	rBV	342564	537444	54.17%	6.501%
25	11.532	3254	3263	3278	rBV5	19995	38316	3.86%	0.463%
26	11.622	3279	3291	3309	rVV	297642	470763	47.45%	5.694%
27	11.956	3385	3395	3404	rBV	10289	16339	1.65%	0.198%
28	12.342	3502	3515	3527	rVB4	11683	19498	1.97%	0.236%
29	12.882	3675	3683	3695	rVB3	16472	24180	2.44%	0.292%
30	13.506	3868	3877	3887	rBV	10735	17551	1.77%	0.212%
31	13.625	3905	3914	3927	rBV2	6519	10640	1.07%	0.129%
32	13.750	3941	3953	3963	rBV2	46977	70605	7.12%	0.854%
33	15.110	4367	4376	4388	rBV4	19601	30150	3.04%	0.365%
34	16.178	4699	4708	4718	rBV4	28506	41996	4.23%	0.508%
35	16.226	4718	4723	4731	rVB5	8648	11821	1.19%	0.143%
36	16.805	4896	4903	4911	rBV10	6852	10833	1.09%	0.131%

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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

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Title : TRACE VOA SFAM1.0

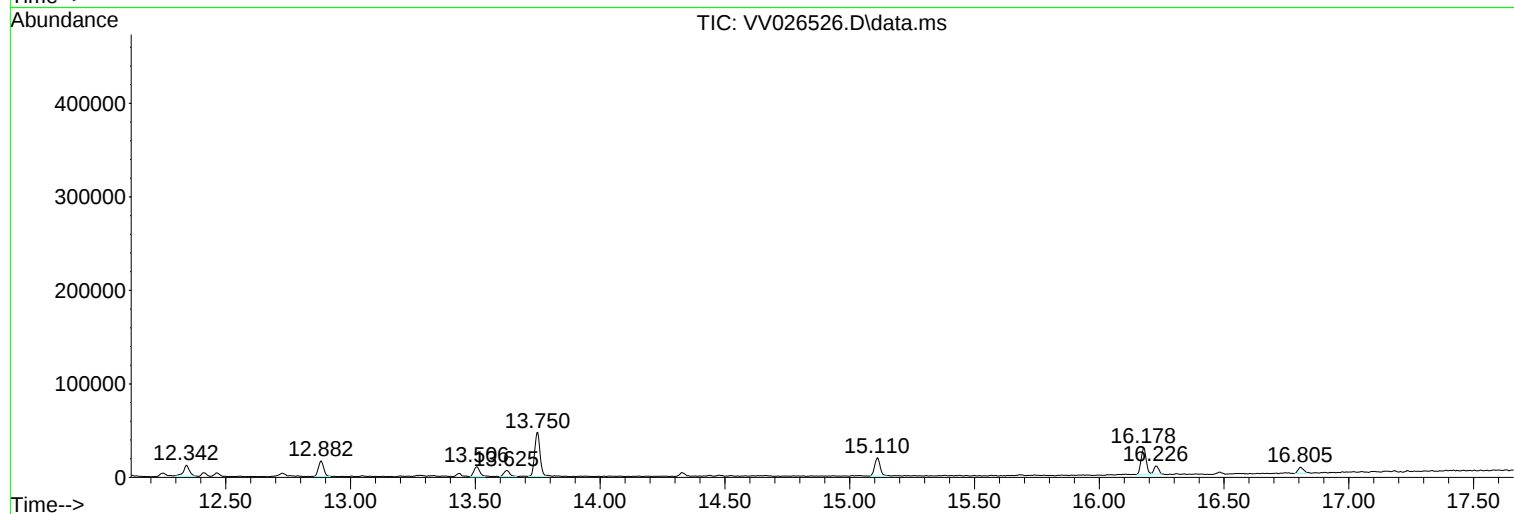
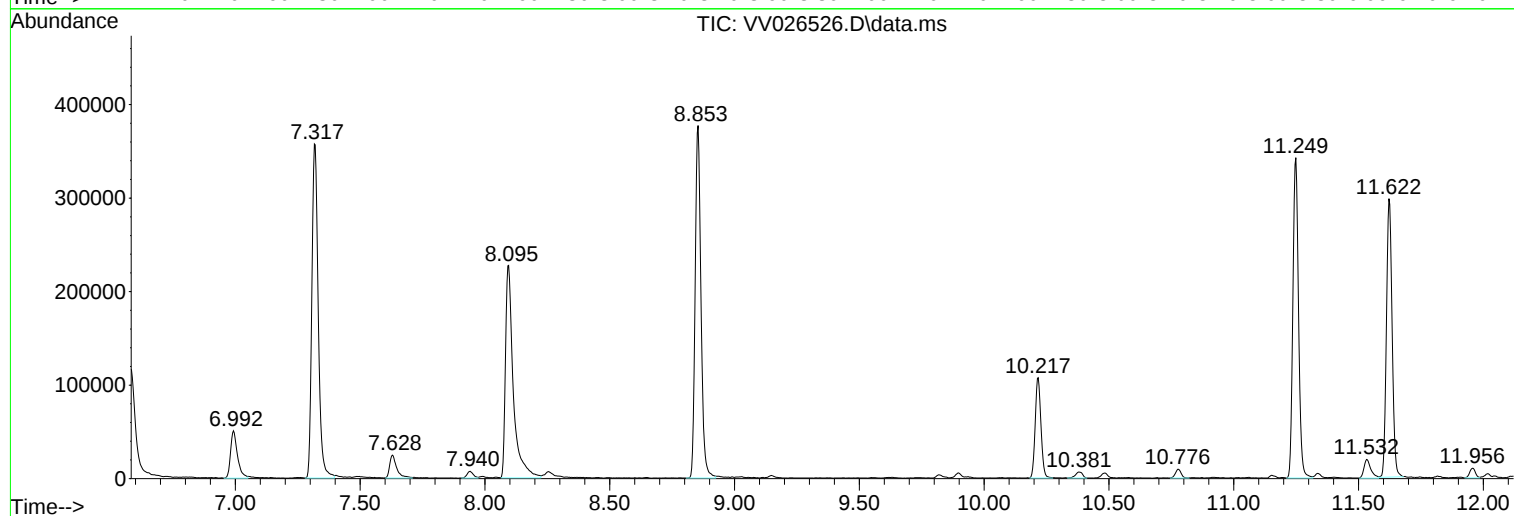
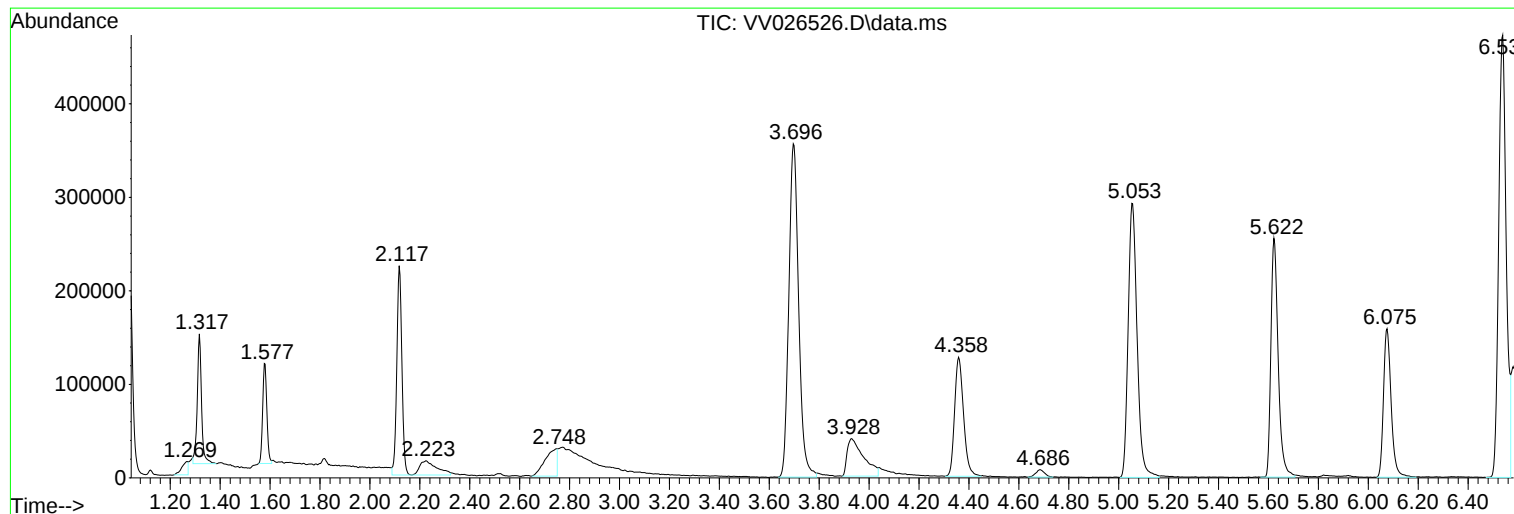
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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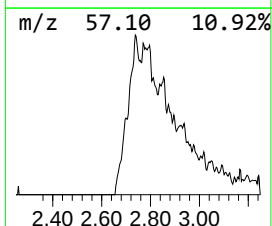
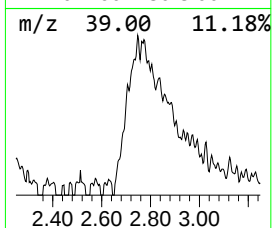
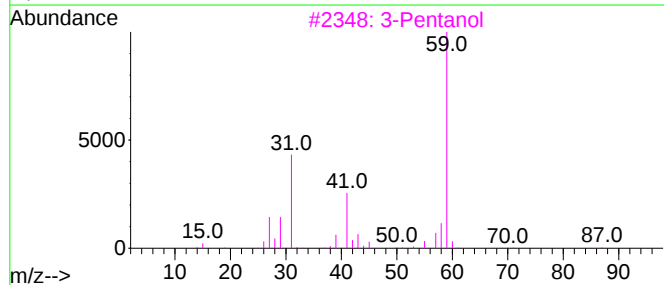
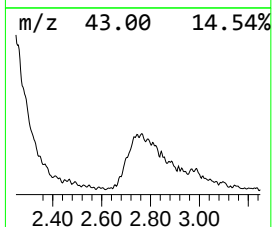
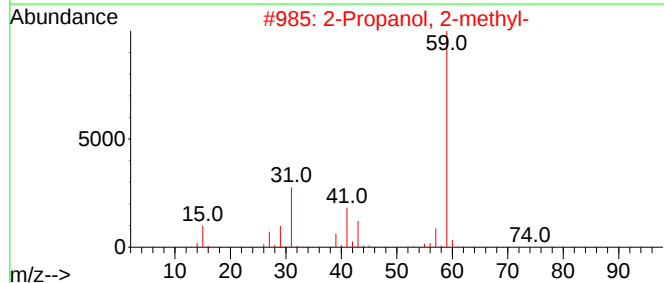
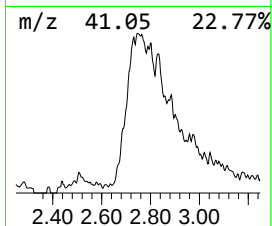
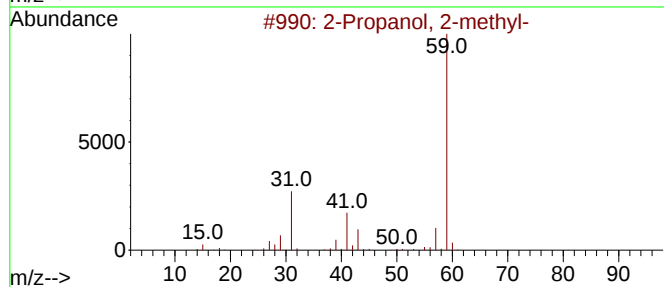
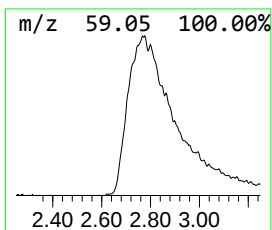
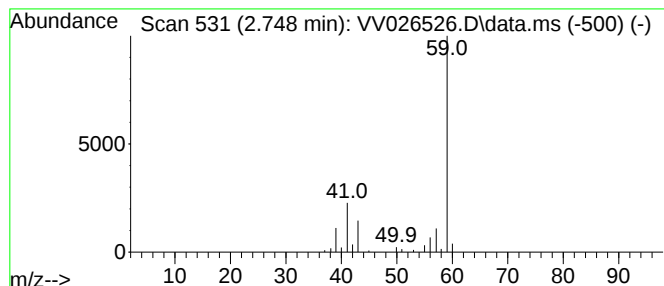
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 2-Propanol, 2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.748	0.96 ug/L	99099	1,4-Difluorobenzene	5.622

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	78
2	2-Propanol, 2-methyl-		74	C4H10O	000075-65-0	64
3	3-Pentanol		88	C5H12O	000584-02-1	40
4	3-Pentanol		88	C5H12O	000584-02-1	9
5	4-Hydroxy-3-hexanone		116	C6H12O2	004984-85-4	9



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ALS Vial : 25 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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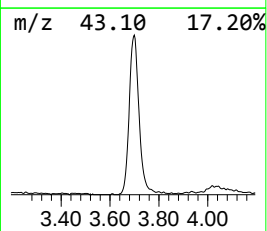
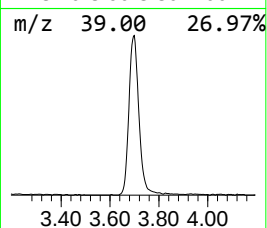
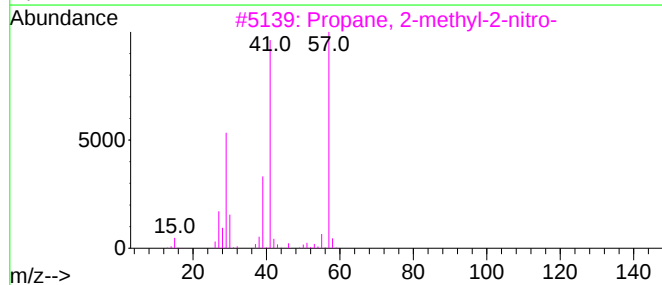
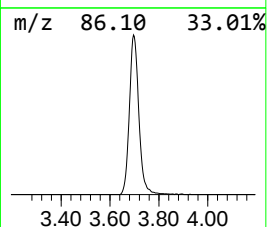
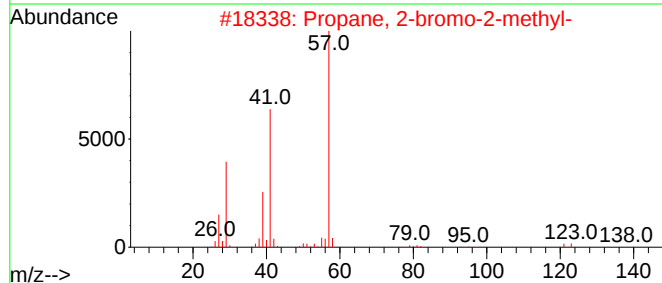
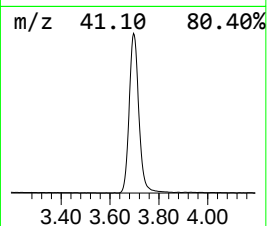
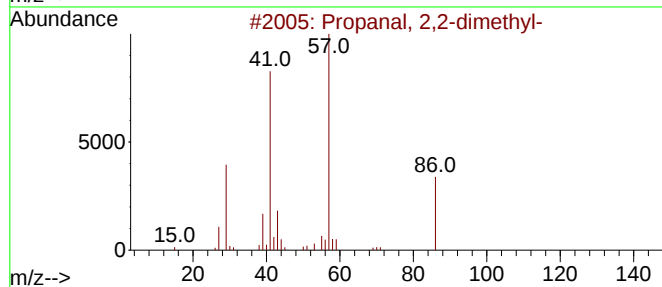
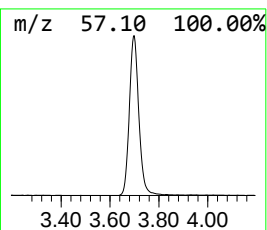
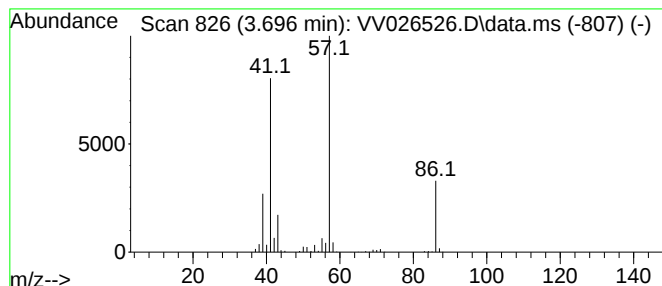
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 Propanal, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.696	9.40 ug/L	973557	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	80
2			Propane, 2-bromo-2-methyl-	136	C4H9Br	000507-19-7	59
3			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	53
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	47
5			3-Heptanone, 5-ethyl-4-methyl-	156	C10H20O	027607-63-2	42



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ALS Vial : 25 Sample Multiplier: 1

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ClientSampleId :
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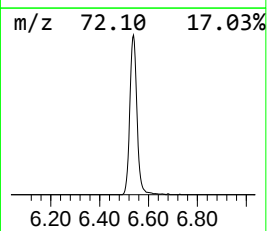
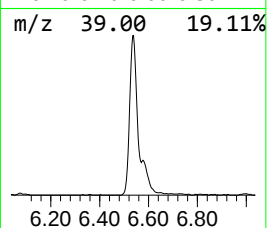
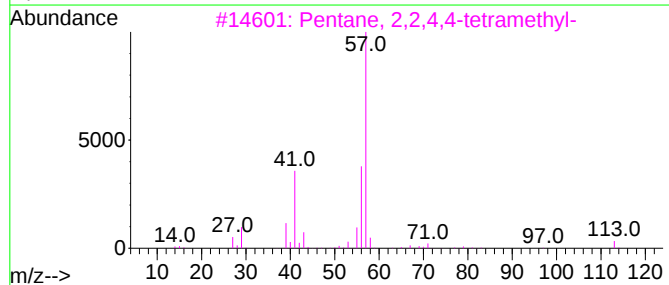
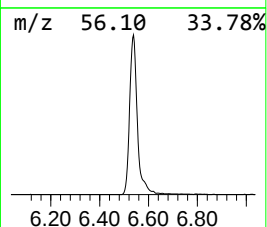
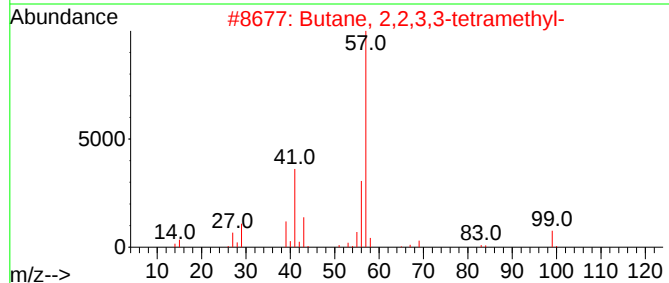
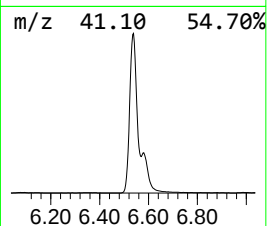
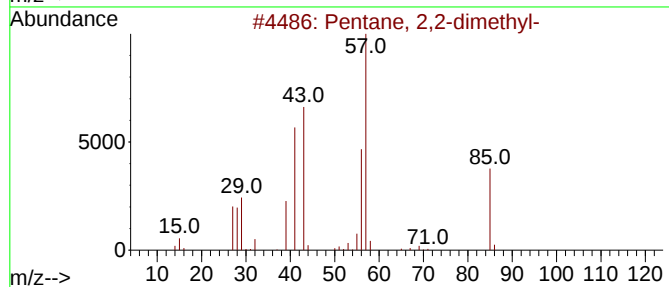
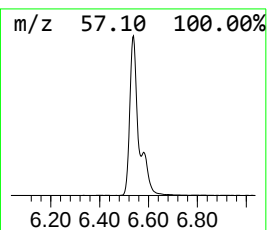
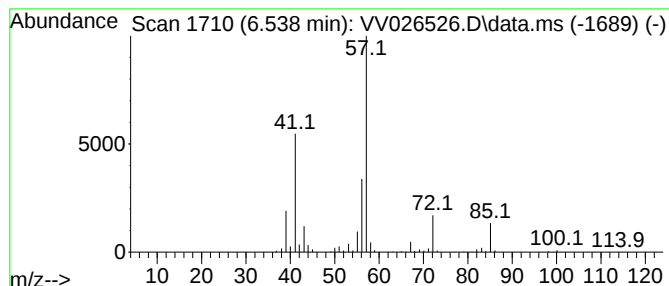
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVTR062322WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 (DEL) Alkane: Straight-Chai... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.538	9.58 ug/L	992064	1,4-Difluorobenzene	5.622

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2-dimethyl-	100	C7H16	000590-35-2	53
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	42
3			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	40
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
5			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38



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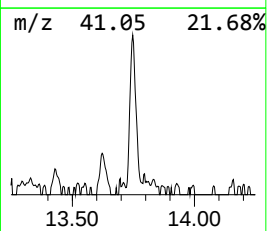
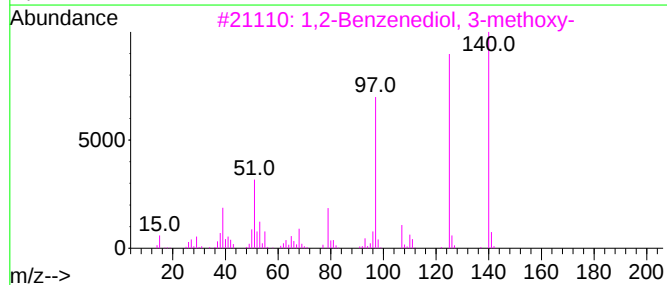
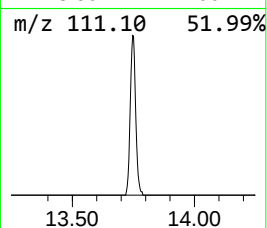
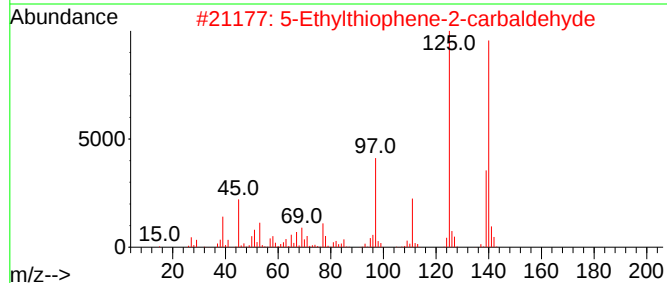
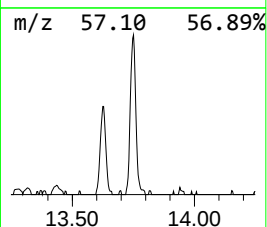
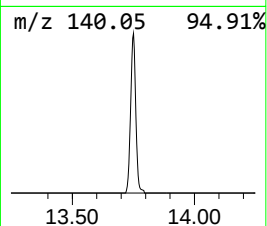
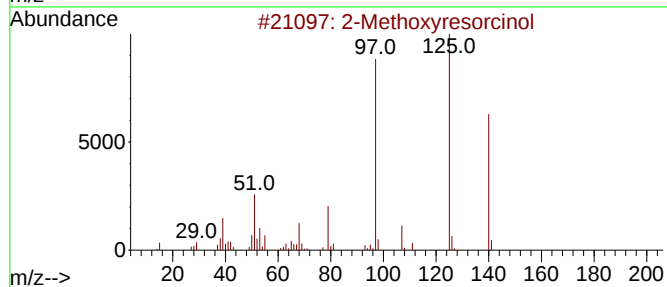
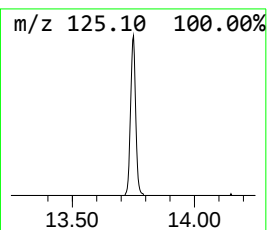
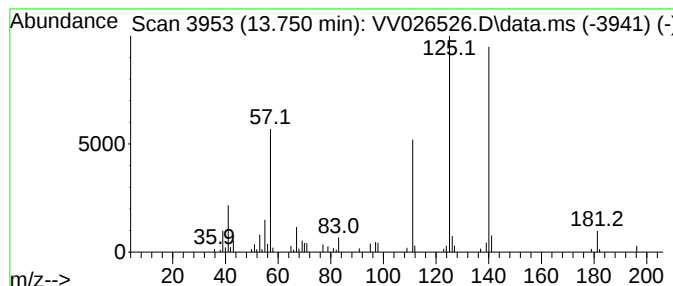
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Methoxyresorcinol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.750	0.66 ug/L	70605	1,4-Dichlorobenzene-d4	11.249

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxyresorcinol	140	C7H8O3	029267-67-2	64
2			5-Ethylthiophene-2-carbaldehyde	140	C7H8OS	036880-33-8	64
3			1,2-Benzenediol, 3-methoxy-	140	C7H8O3	000934-00-9	59
4			Benzenethiol, 4-methoxy-	140	C7H8OS	000696-63-9	59
5			1,4-Benzenediol, 2-methoxy-	140	C7H8O3	000824-46-4	59



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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
2-Propanol, 2-m...	2.748	1.0	ug/L	99099	1	5.622	517764	5.0
Propanal, 2,2-d...	3.696	9.4	ug/L	973557	1	5.622	517764	5.0
(DEL) Alkane: S...	6.538	9.6	ug/L	992064	1	5.622	517764	5.0
2-Methoxyresorc...	13.750	0.7	ug/L	70605	3	11.249	537444	5.0