

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
 Data File : VU060432.D
 Acq On : 13 Aug 2024 18:08
 Operator : MD/SY
 Sample : P3501-15
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0BX2

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_U\Method\SFAMUTR080824WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU060432.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.596	84	95	109	rVB2	30954	45332	14.50%	1.696%
2	1.908	182	192	208	rBV	30083	41835	13.38%	1.565%
3	2.560	384	395	411	rVB	51215	81970	26.22%	3.066%
4	2.644	411	421	460	rBV2	14208	43587	13.94%	1.631%
5	3.229	580	603	605	rBV3	5481	13508	4.32%	0.505%
6	4.432	964	977	992	rBV4	8262	21086	6.74%	0.789%
7	4.634	1026	1040	1075	rBV	43030	143099	45.77%	5.353%
8	5.055	1157	1171	1192	rBV3	60503	135063	43.20%	5.052%
9	5.718	1359	1377	1402	rBV3	109918	293947	94.02%	10.996%
10	6.242	1529	1540	1565	rBV	94273	185010	59.18%	6.921%
11	6.685	1664	1678	1701	rBV	72938	146370	46.82%	5.475%
12	7.155	1805	1824	1846	rBV3	11712	28957	9.26%	1.083%
13	7.560	1940	1950	1969	rBV2	29209	51787	16.56%	1.937%
14	7.894	2041	2054	2076	rBV	116445	212572	67.99%	7.952%
15	8.177	2133	2142	2158	rBV	17128	29900	9.56%	1.119%
16	8.467	2222	2232	2246	rVB4	7764	14554	4.66%	0.544%
17	8.628	2269	2282	2297	rBV	162622	312646	100.00%	11.696%
18	9.412	2514	2526	2549	rBV	139669	246753	78.92%	9.231%
19	10.750	2930	2942	2958	rBV	61541	101211	32.37%	3.786%
20	10.888	2973	2985	2996	rBV	23412	38186	12.21%	1.428%
21	11.576	3190	3199	3210	rVB3	6689	9752	3.12%	0.365%
22	11.807	3256	3271	3288	rBV	132018	218552	69.90%	8.176%
23	11.888	3288	3296	3311	rVB5	12149	22340	7.15%	0.836%
24	12.187	3375	3389	3405	rBV	122726	207636	66.41%	7.767%
25	12.766	3558	3569	3581	rBV2	7663	12054	3.86%	0.451%
26	13.377	3751	3759	3772	rBV3	7057	11683	3.74%	0.437%
27	14.573	4122	4131	4139	rVB	2559	3826	1.22%	0.143%

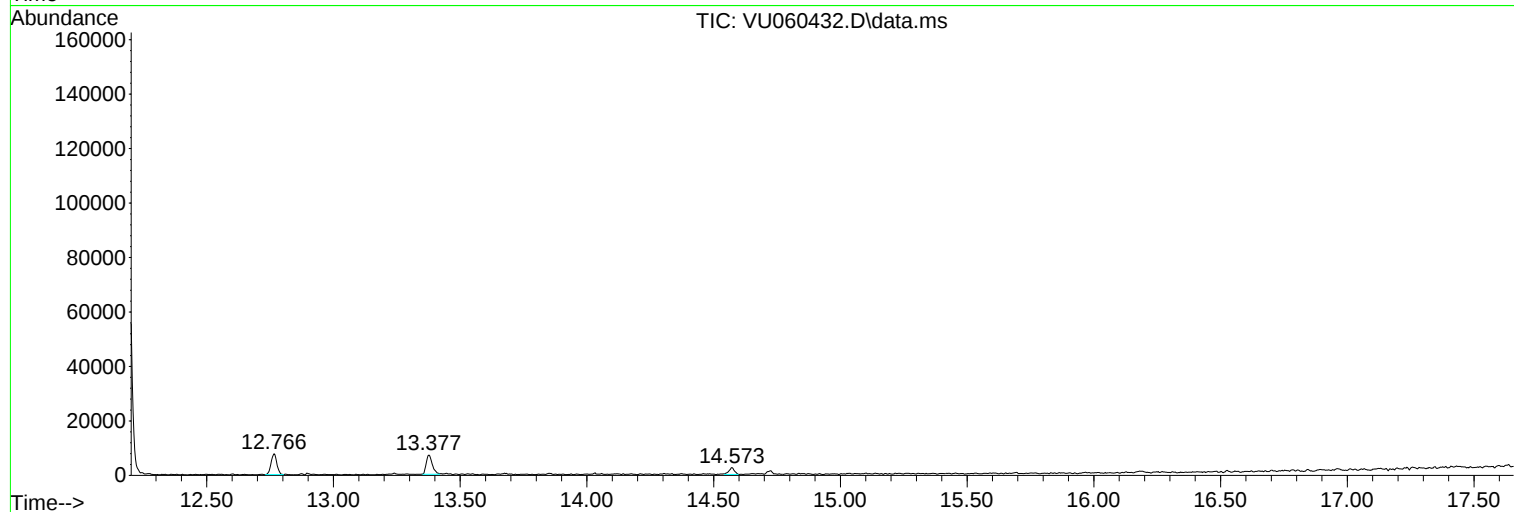
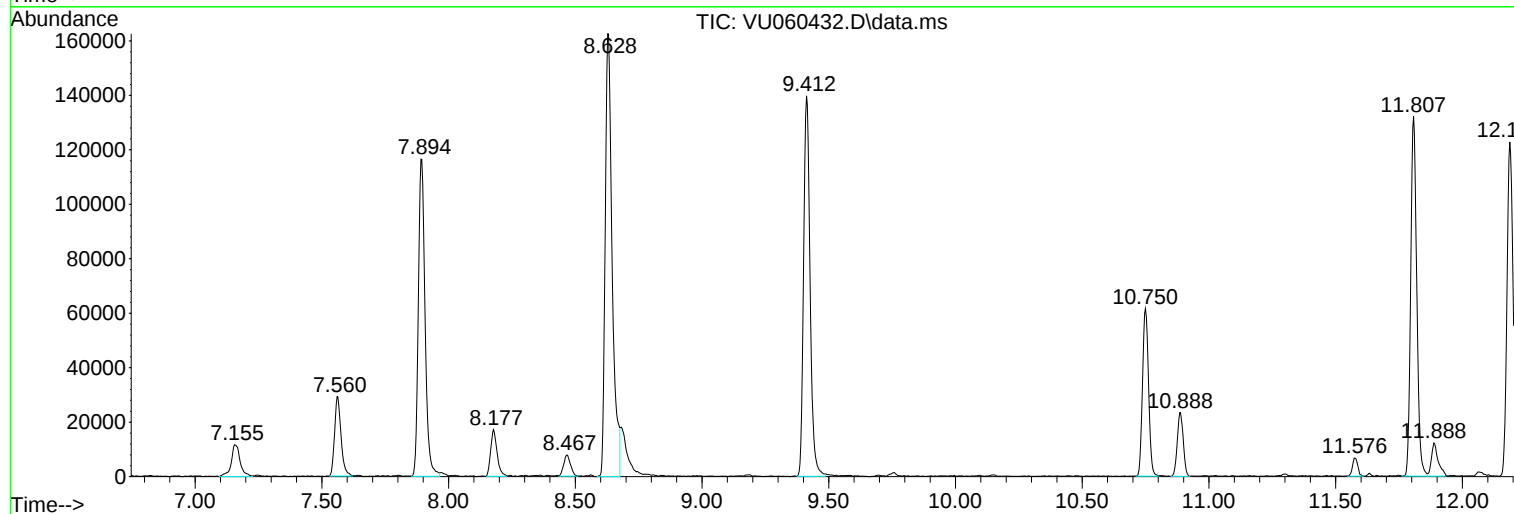
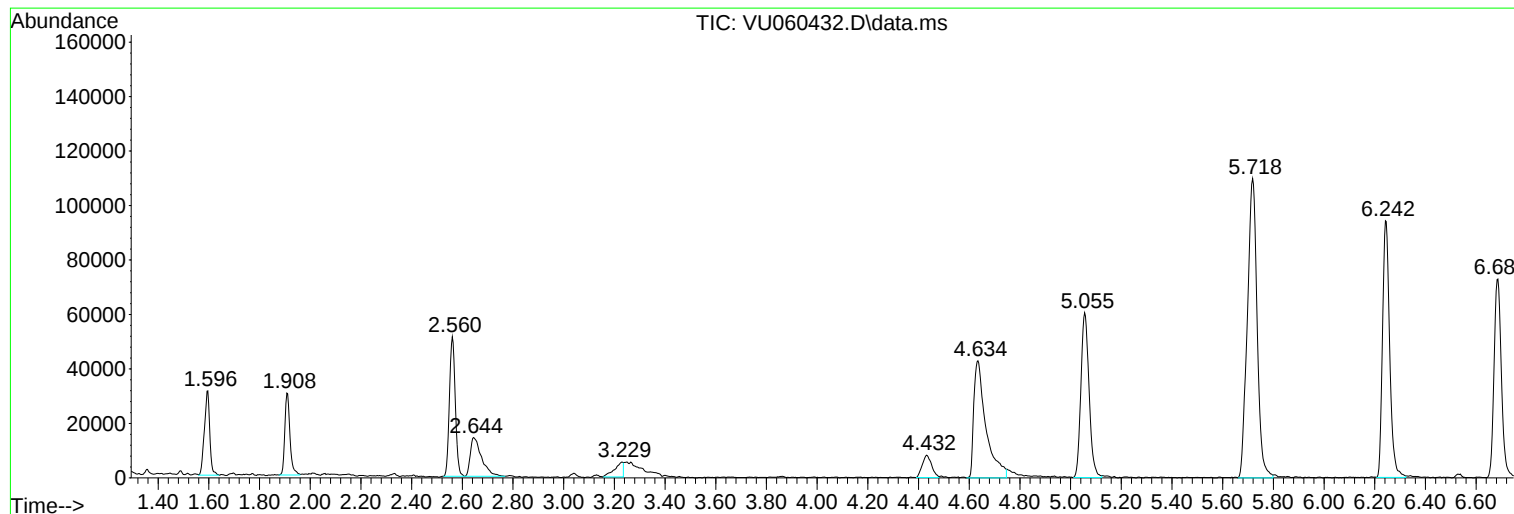
Sum of corrected areas: 2673216

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
Data File : VU060432.D
Acq On : 13 Aug 2024 18:08
Operator : MD/SY
Sample : P3501-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080824WMA.M
Quant Title : TRACE VOA SFAM1.0

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
Data File : VU060432.D
Acq On : 13 Aug 2024 18:08
Operator : MD/SY
Sample : P3501-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BX2

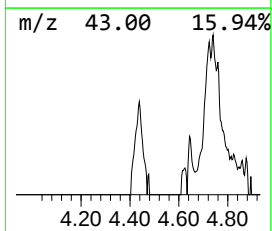
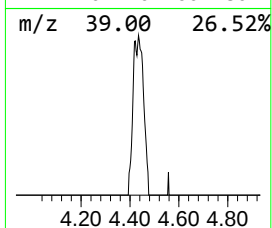
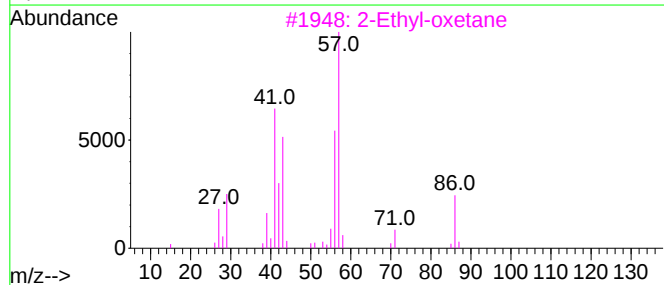
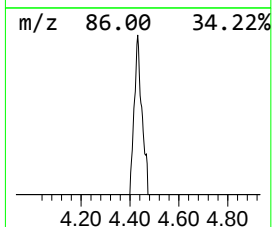
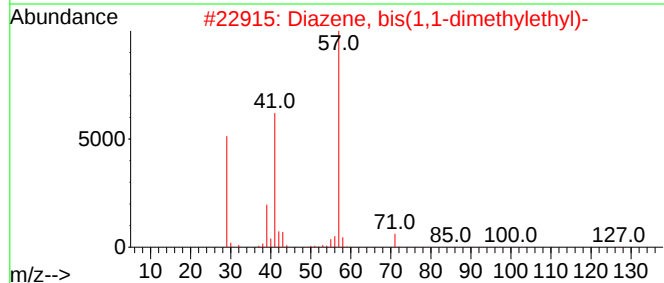
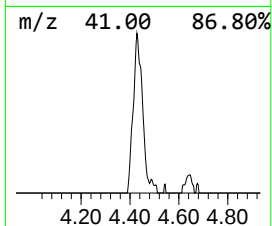
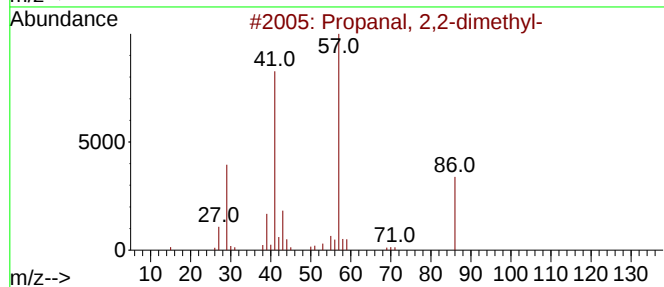
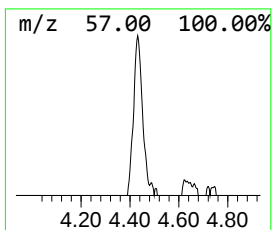
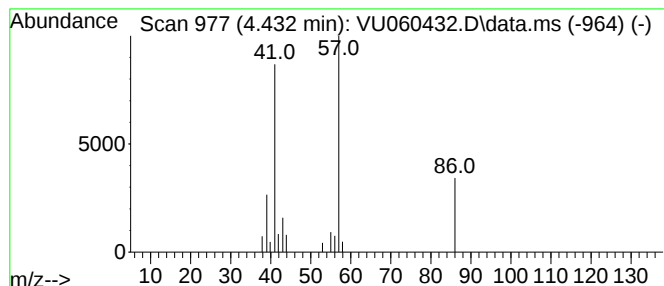
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 Propanal, 2,2-dimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.432	0.57 ug/L	21086	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanal, 2,2-dimethyl-	86	C5H10O	000630-19-3	90
2			Diazene, bis(1,1-dimethylethyl)-	142	C8H18N2	000927-83-3	50
3			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	45
4			Propane, 2-methyl-2-nitro-	103	C4H9NO2	000594-70-7	40
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
Data File : VU060432.D
Acq On : 13 Aug 2024 18:08
Operator : MD/SY
Sample : P3501-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BX2

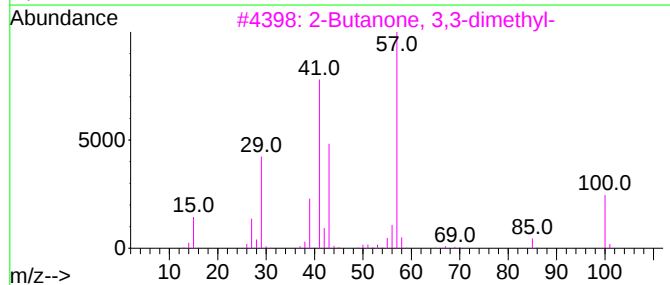
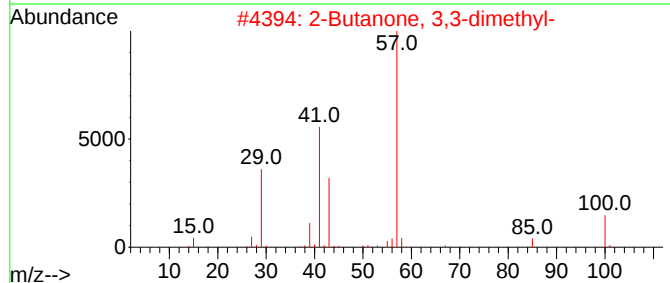
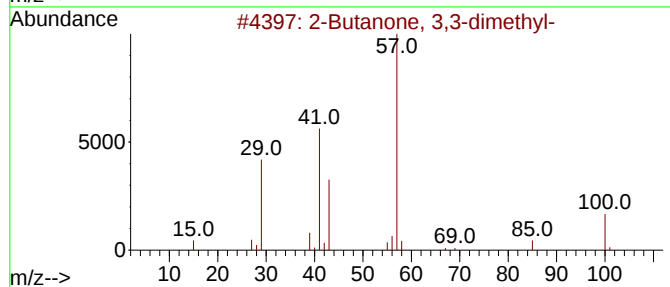
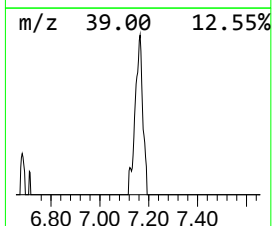
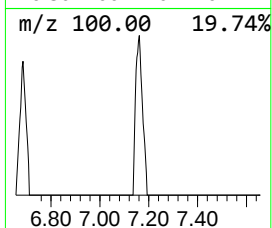
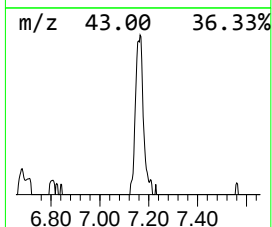
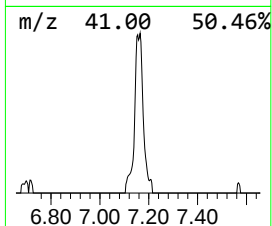
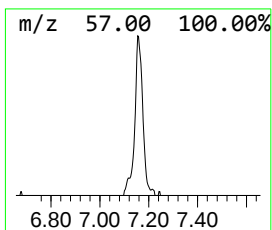
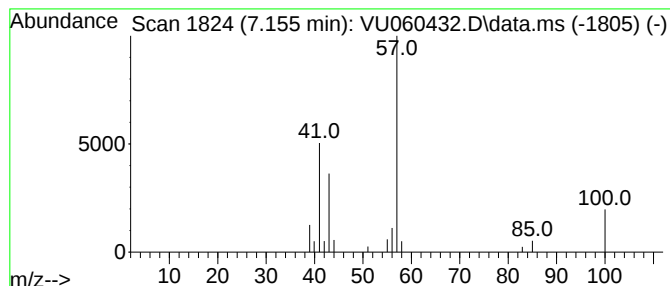
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 2 2-Butanone, 3,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.155	0.78 ug/L	28957	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	90	
2	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	72	
3	2-Butanone, 3,3-dimethyl-		100	C6H12O	000075-97-8	72	
4	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	42	
5	3-Pentanone, 2-methyl-		100	C6H12O	000565-69-5	42	



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
Data File : VU060432.D
Acq On : 13 Aug 2024 18:08
Operator : MD/SY
Sample : P3501-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BX2

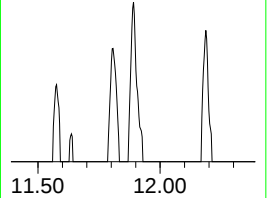
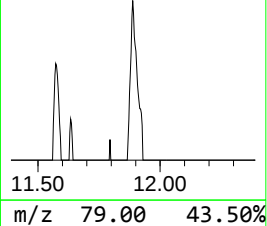
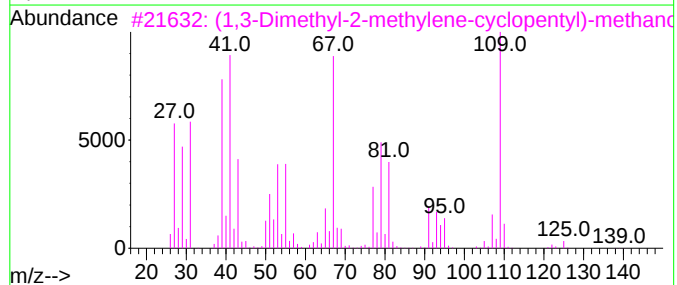
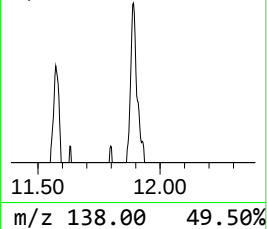
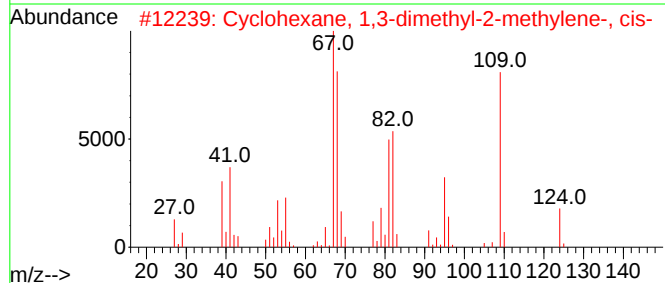
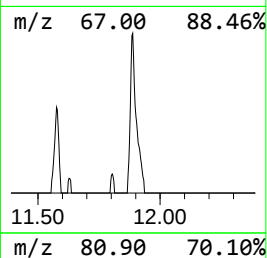
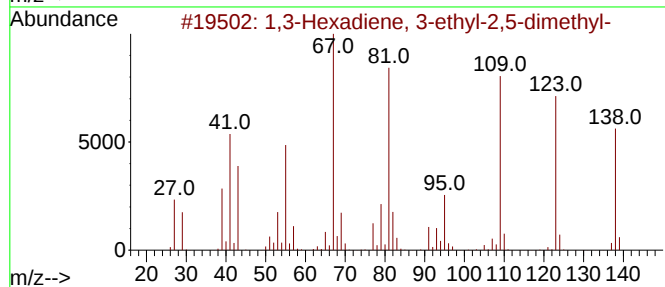
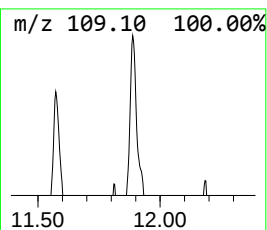
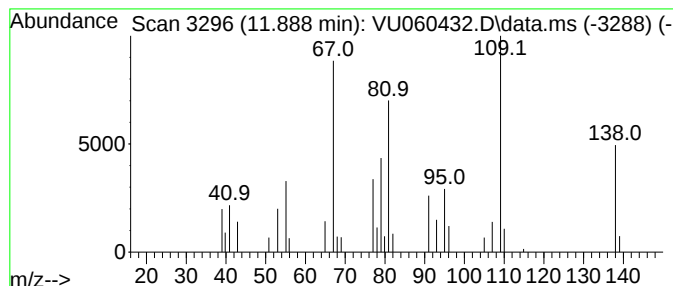
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080824WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 5 1,3-Hexadiene, 3-ethyl-2,5-... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.888	0.51 ug/L	22340	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Hexadiene, 3-ethyl-2,5-dimet...	138	C10H18	062338-07-2	76
2			Cyclohexane, 1,3-dimethyl-2-meth...	124	C9H16	019781-47-6	53
3			(1,3-Dimethyl-2-methylene-cyclop...	140	C9H16O	1000190-16-2	50
4			Cyclopentanone, 2-(2-methylpropy...	138	C9H14O	016856-72-7	46
5			Naphthalene, decahydro-, cis-	138	C10H18	000493-01-6	43



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU081324\
Data File : VU060432.D
Acq On : 13 Aug 2024 18:08
Operator : MD/SY
Sample : P3501-15
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BX2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR080824WMA.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
Propanal, 2,2-d...	4.432	0.6	ug/L	21086	1	6.245	185010	5.0
2-Butanone, 3,3...	7.155	0.8	ug/L	28957	1	6.245	185010	5.0
1,3-Hexadiene, ...	11.888	0.5	ug/L	22340	3	11.807	218552	5.0