

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
 Data File : VU057713.D
 Acq On : 29 Jan 2024 13:41
 Operator : MD/SY
 Sample : P1230-06
 Misc : 25.0mL/MSVOA_U/WATER
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0BF4

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\SFAMUTR012324WMA.M
 Title : TRACE VOA SFAM1.0

Signal : TIC: VU057713.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.355	15	20	25	rBV	3253	2886	1.42%	0.149%
2	1.596	85	95	108	rVB	30668	38753	19.03%	2.001%
3	1.689	117	124	134	rBV2	1641	2065	1.01%	0.107%
4	1.911	185	193	207	rBV	22611	30263	14.86%	1.563%
5	2.432	343	355	356	rBV3	2498	3834	1.88%	0.198%
6	2.563	386	396	411	rVB	48849	82400	40.46%	4.255%
7	4.432	961	977	988	rBV4	3906	10441	5.13%	0.539%
8	4.631	1028	1039	1083	rBV	20134	63898	31.38%	3.300%
9	5.055	1157	1171	1192	rBV	39562	87981	43.20%	4.544%
10	5.718	1359	1377	1403	rBV2	81127	203650	100.00%	10.517%
11	6.242	1523	1540	1562	rBV	86353	164136	80.60%	8.476%
12	6.686	1666	1678	1698	rVB	48204	92740	45.54%	4.789%
13	7.120	1799	1813	1837	rVB3	13448	29826	14.65%	1.540%
14	7.560	1936	1950	1968	rBV2	24749	43567	21.39%	2.250%
15	7.894	2041	2054	2070	rBV	101185	177773	87.29%	9.181%
16	7.965	2070	2076	2088	rVB2	2217	4324	2.12%	0.223%
17	8.174	2131	2141	2161	rBV	13484	23355	11.47%	1.206%
18	8.631	2272	2283	2321	rBV3	83869	175063	85.96%	9.041%
19	8.782	2321	2330	2355	rVB2	14343	27533	13.52%	1.422%
20	9.412	2515	2526	2554	rBV	115229	196745	96.61%	10.160%
21	9.570	2567	2575	2581	rBV	1615	2094	1.03%	0.108%
22	9.689	2603	2612	2624	rBV	5082	8310	4.08%	0.429%
23	10.103	2731	2741	2754	rBV5	2234	4276	2.10%	0.221%
24	10.345	2802	2816	2826	rBV4	2788	5860	2.88%	0.303%
25	10.750	2932	2942	2957	rVB	29816	47859	23.50%	2.472%
26	10.898	2981	2988	3000	rBV3	2047	3875	1.90%	0.200%
27	11.528	3178	3184	3194	rVB3	5301	7543	3.70%	0.390%
28	11.685	3227	3233	3242	rVB3	1656	2214	1.09%	0.114%
29	11.807	3260	3271	3289	rBV	117001	184123	90.41%	9.509%
30	12.058	3340	3349	3366	rBV2	5008	10262	5.04%	0.530%
31	12.187	3378	3389	3408	rBV	86010	138767	68.14%	7.166%
32	12.524	3483	3494	3512	rBV	22324	35352	17.36%	1.826%
33	12.885	3594	3606	3617	rBV3	7842	11956	5.87%	0.617%
34	14.309	4043	4049	4057	rBV	1857	2490	1.22%	0.129%
35	14.479	4095	4102	4111	rVB3	2136	3216	1.58%	0.166%
36	15.688	4470	4478	4485	rBV3	5487	6962	3.42%	0.360%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

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\SFAMUTR012324WMA.M
Title : TRACE VOA SFAM1.0

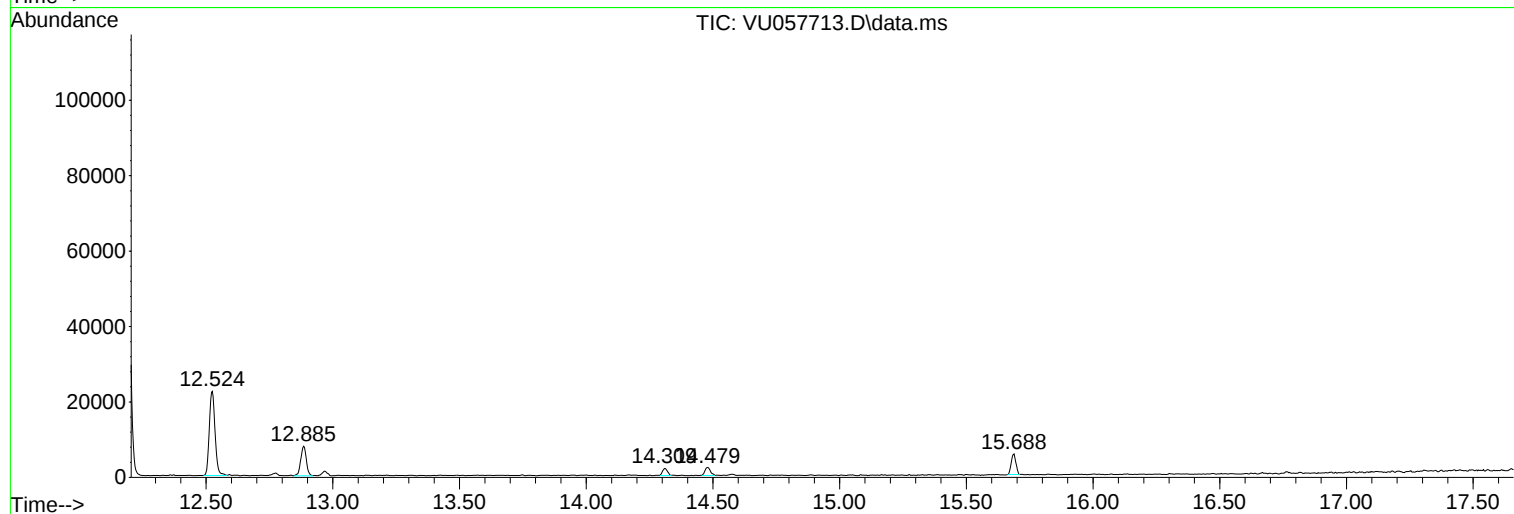
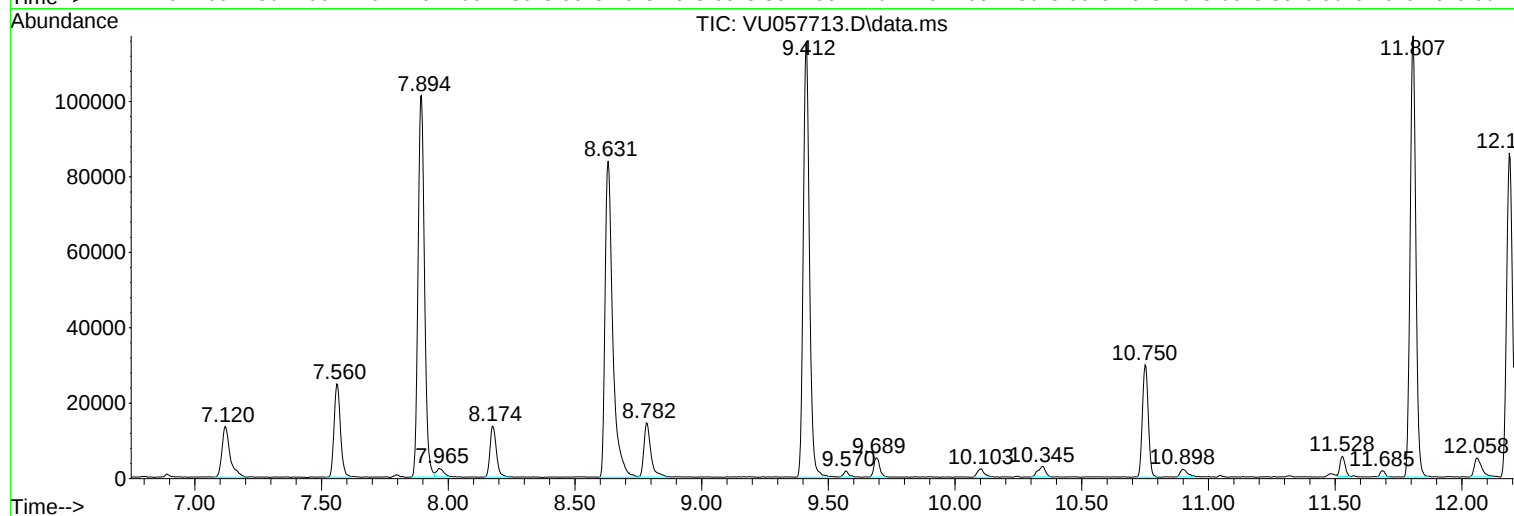
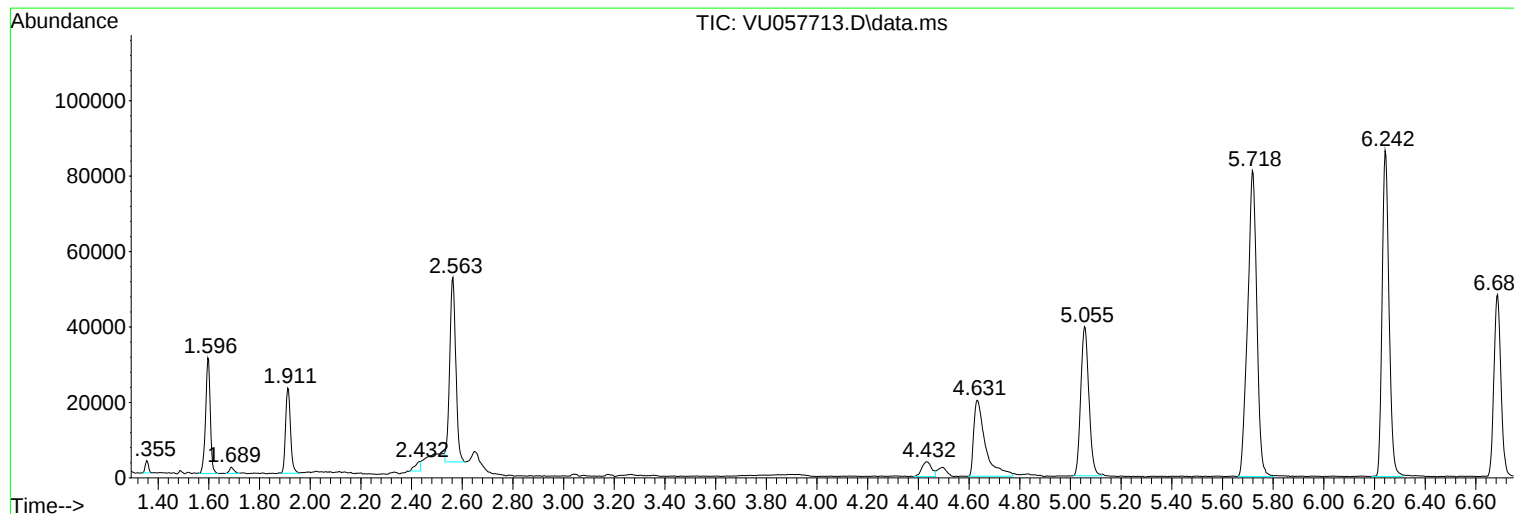
Sum of corrected areas: 1936392

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.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\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

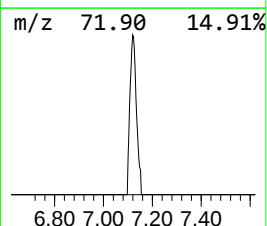
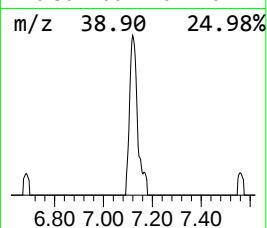
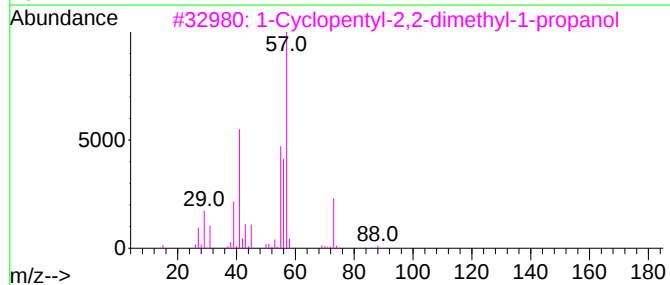
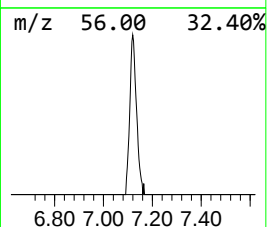
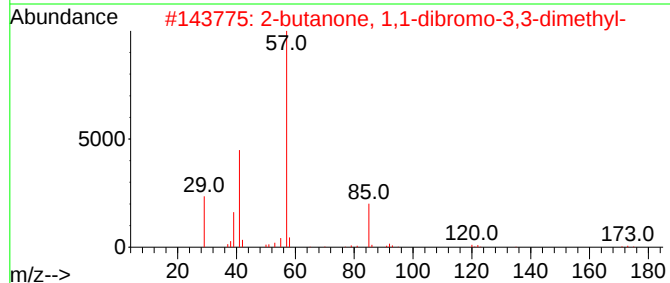
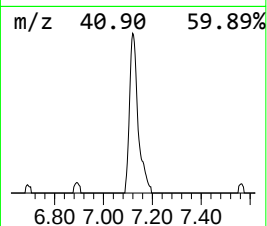
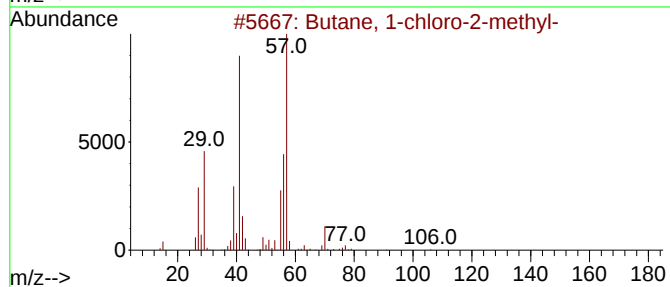
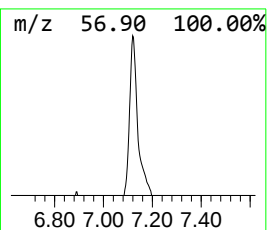
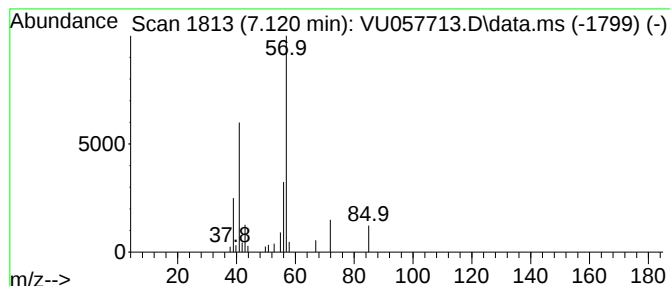
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.120	0.91 ug/L	29826	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 1-chloro-2-methyl-	106	C5H11Cl	000616-13-7	40
2			2-butanone, 1,1-dibromo-3,3-dime...	256	C6H10Br2O	1000401-51-7	38
3			1-Cyclopentyl-2,2-dimethyl-1-pro...	156	C10H20O	337966-85-5	36
4			1-Butanesulfonyl chloride	156	C4H9ClO2S	002386-60-9	36
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	36



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

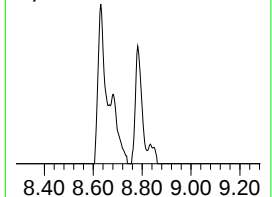
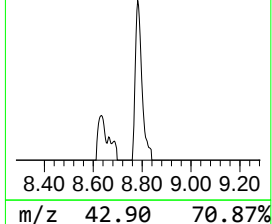
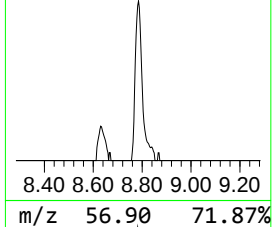
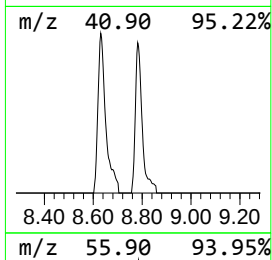
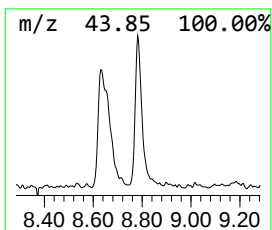
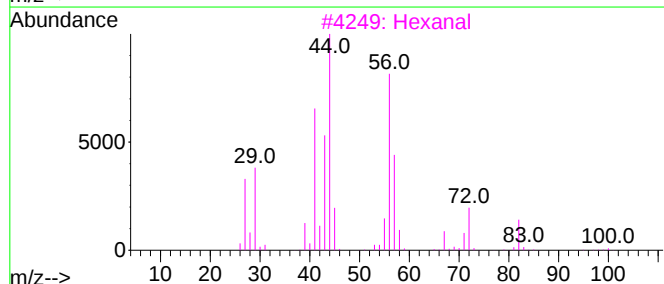
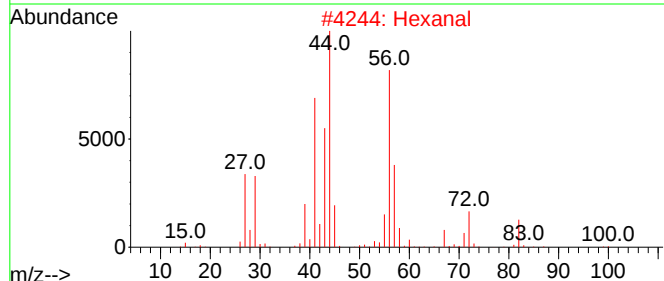
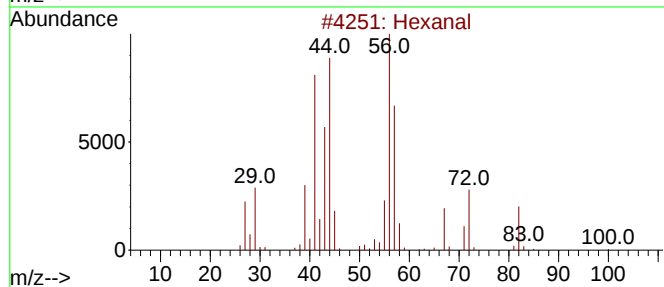
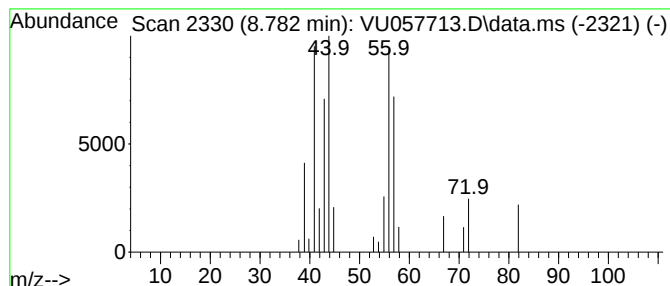
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 3 Hexanal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.782	0.70 ug/L	27533	Chlorobenzene-d5	9.412

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanal			100	C6H12O	000066-25-1	72
2	Hexanal			100	C6H12O	000066-25-1	64
3	Hexanal			100	C6H12O	000066-25-1	64
4	Hexanal			100	C6H12O	000066-25-1	64
5	Hexanal			100	C6H12O	000066-25-1	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

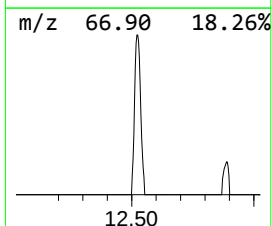
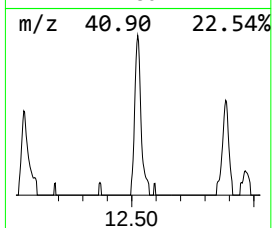
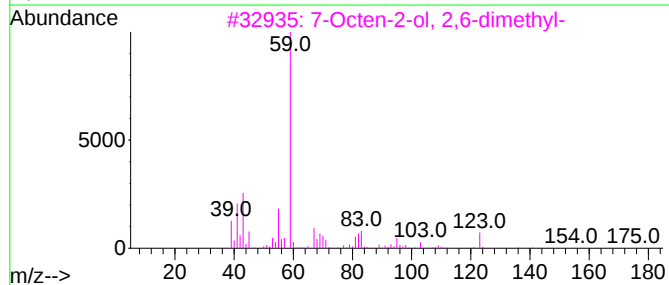
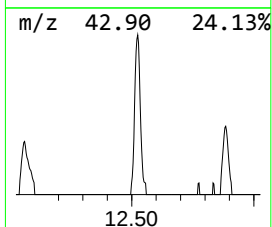
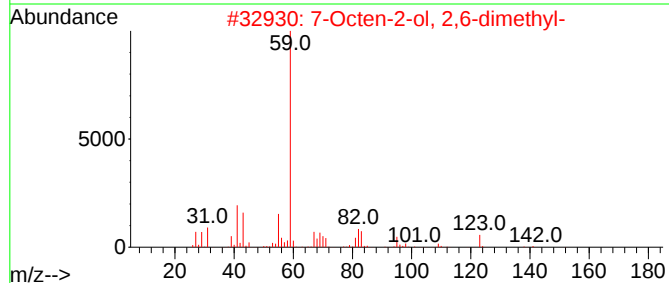
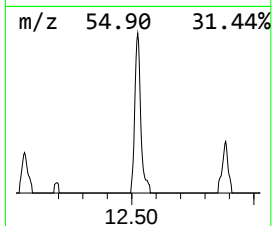
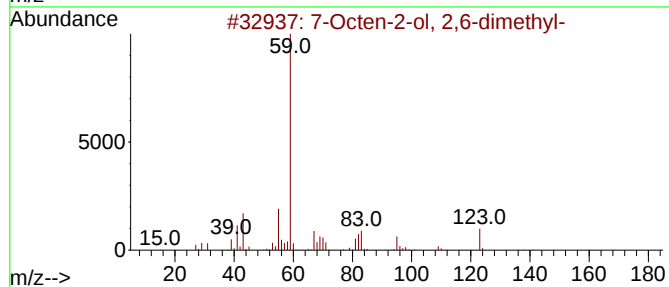
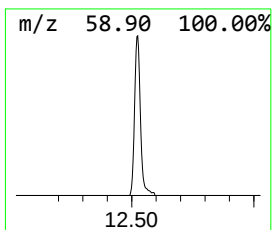
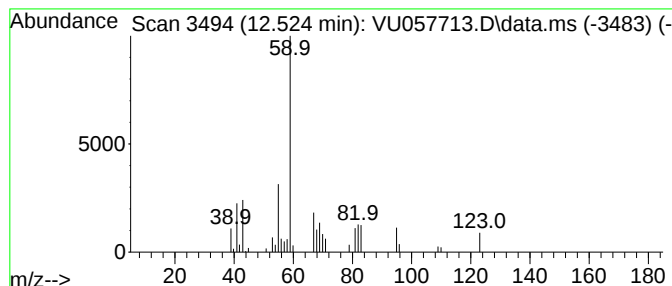
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.M
Quant Title : TRACE VOA SFAM1.0

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

Peak Number 4 7-Octen-2-ol, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.525	0.96 ug/L	35352	1,4-Dichlorobenzene-d4	11.807

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	83
2			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
3			7-Octen-2-ol, 2,6-dimethyl-	156	C10H20O	018479-58-8	64
4			Cyclopentanemethanol, .alpha.,.a...	128	C8H16O	001462-06-2	59
5			2-Octanol, 2-methyl-6-methylene-	156	C10H20O	018479-59-9	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU012924\
Data File : VU057713.D
Acq On : 29 Jan 2024 13:41
Operator : MD/SY
Sample : P1230-06
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0BF4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR012324WMA.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
unknown-01	7.120	0.9	ug/L	29826	1	6.242	164136	5.0
Hexanal	8.782	0.7	ug/L	27533	2	9.412	196745	5.0
7-Octen-2-ol, 2...	12.525	1.0	ug/L	35352	3	11.807	184123	5.0