Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

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\SFAMUTR100124WMA.M
Title : TRACE VOA SFAM1.0

Signal : TIC: VU061097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.358	12	21	36	rBV2	58416	67951	5.91%	0.928%
2	1.470	49	56	66	rBV	197806	209387	18.20%	2.861%
3	1.593	83	94	107	rBV3	103878	148588	12.92%	2.030%
4	1.724	127	135	149	rVB	170073	210680	18.31%	2.879%
5	1.908	184	192	203	rVB	46749	62378	5.42%	0.852%
6	1.988	210	217	229	rVB	20033	27349	2.38%	0.374%
7	2.194	275	281	293	rVB2	16857	24275	2.11%	0.332%
8	2.557	383	394	408	rVB	93082	151705	13.19%	2.073%
9	2.673	415	430	452	rBV3	10183	29608	2.57%	0.405%
10	3.355	624	642	655	rVB5	4825	13281	1.15%	0.181%
11	4.647	1028	1044	1096	rBV2	49243	212884	18.51%	2.909%
12	5.052	1155	1170	1196	rBV	88163	200236	17.41%	2.736%
13	5.715	1355	1376	1408	rBV2	181479	510099	44.34%	6.970%
14	6.239	1527	1539	1567	rBV	205730	407554	35.43%	5.568%
15	6.682	1664	1677	1693	rBV	113357	226341	19.68%	3.093%
16	7.560	1937	1950	1976	rBV	60447	113768	9.89%	1.554%
17	7.891	2040	2053	2068	rBV	220155	394509	34.29%	5.390%
18	7.962	2068	2075	2087	rVB2	24372	43617	3.79%	0.596%
19	8.174	2129	2141	2158	rBV	35569	66077	5.74%	0.903%
20	8.547	2248	2257	2270	rVB2	10607	17534	1.52%	0.240%
21	8.628	2270	2282	2322	rBV	250097	534060	46.43%	7.297%
22	9.409	2514	2525	2561	rVB	286842	501622	43.61%	6.854%
23	9.689	2601	2612	2626	rBV	32146	56953	4.95%	0.778%
24	10.094	2728	2738	2751	rBV	25230	42319	3.68%	0.578%
25	10.477	2847	2857	2870	rBV	19331	31567	2.74%	0.431%
26	10.747	2930	2941	2960	rBV	83804	137476	11.95%	1.878%
27	11.081	3036	3045	3068	rVB	45087	73651	6.40%	1.006%
28	11.287	3100	3109	3120	rVB	7561	12004	1.04%	0.164%
29	11.464	3155	3164	3190	rVB3	16422	38366	3.34%	0.524%
30	11.737	3239	3249	3257	rBV2	17412	26812	2.33%	0.366%
31	11.804	3257	3270	3286	rVV	305615	513301	44.62%	7.013%
32	11.888	3287	3296	3310	rVB	28712	46421	4.04%	0.634%
33	12.001	3319	3331	3340	rBV	47246	73069	6.35%	0.998%
34	12.058	3340	3349	3377	rVV3	33775	104769	9.11%	1.431%
35	12.184	3377	3388	3409	rVB	219681	368390	32.02%	5.033%
36	12.602	3510	3518	3528	rVB	25216	37779	3.28%	0.516%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

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\SFAMUTR100124WMA.M
Title : TRACE VOA SFAM1.0

37	12.869	3592	3601	3613	rVB4	6594	12625	1.10%	0.172%
38	12.936	3613	3622	3627	rBV3	8147	12692	1.10%	0.173%
39	13.020	3639	3648	3664	rVB2	23558	39736	3.45%	0.543%
40	13.103	3664	3674	3685	rBV3	8120	13091	1.14%	0.179%
41	13.441	3763	3779	3792	rVB5	23841	45586	3.96%	0.623%
42	14.078	3963	3977	4003	rBV	688879	1150354	100.00%	15.718%
43	14.203	4006	4016	4025	rVB	13092	22322	1.94%	0.305%
44	15.216	4321	4331	4352	rBV	65136	108604	9.44%	1.484%
45	15.402	4377	4389	4403	rBV	44165	74717	6.50%	1.021%
46	15.952	4550	4560	4576	rVB3	10276	18884	1.64%	0.258%
47	16.261	4645	4656	4664	rBV3	8579	15100	1.31%	0.206%
48	16.406	4691	4701	4708	rBV3	14528	24622	2.14%	0.336%
49	16.444	4708	4713	4724	rVB3	7603	11940	1.04%	0.163%
50	16.885	4841	4850	4861	rBV2	10317	17903	1.56%	0.245%
51	17.090	4906	4914	4924	rBV2	8382	14365	1.25%	0.196%

Sum of corrected areas: 7318921

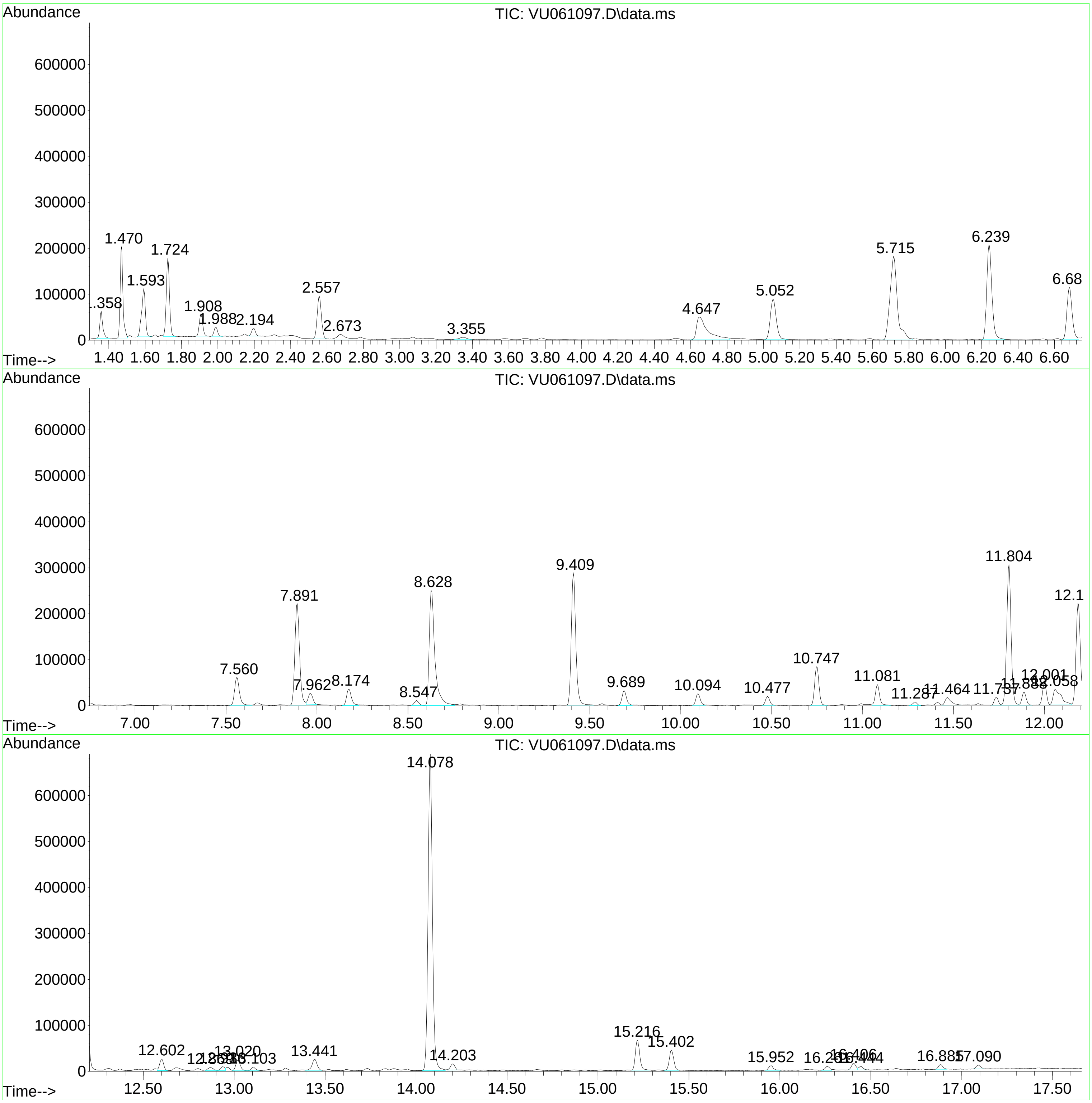
LSC Report - Integrated Chromatogram

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

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



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Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On    : 10 Oct 2024  18:24
Operator  : MD/SY
Sample    : P4380-13
Misc      : 25.0mL/MSVOA_U/WATER
ALS Vial  : 18   Sample Multiplier: 1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title  : TRACE VOA SFAM1.0

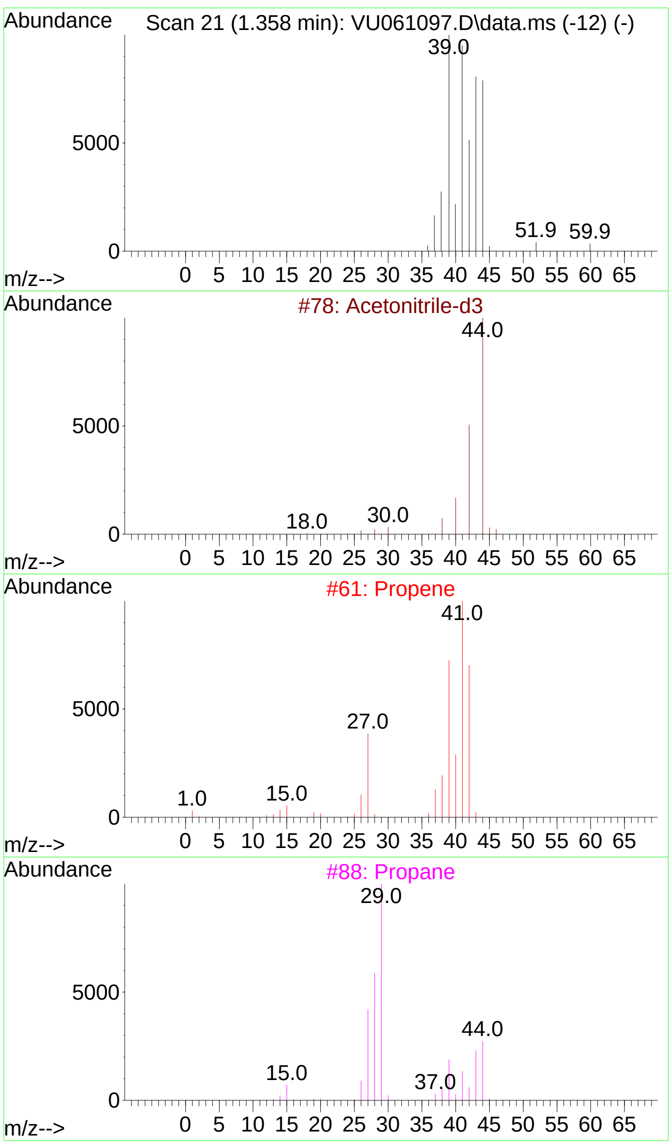
TIC Library    : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P
```

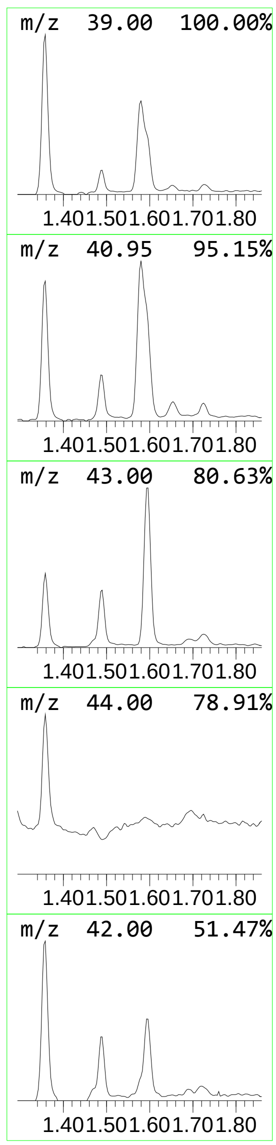
Instrument :
MSVOA_U
ClientSampleId :
E27H2

```
**********************************************************************
Peak Number  1  unknown-01                      Concentration Rank  7
```

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.358	0.83 ug/L	67951	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetonitrile-d3	44	C2D3N	002206-26-0	7
2	Propene	42	C3H6	000115-07-1	7
3	Propane	44	C3H8	000074-98-6	5
4	Cyclopropane	42	C3H6	000075-19-4	4
5	Cyclopropene	40	C3H4	002781-85-3	4





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

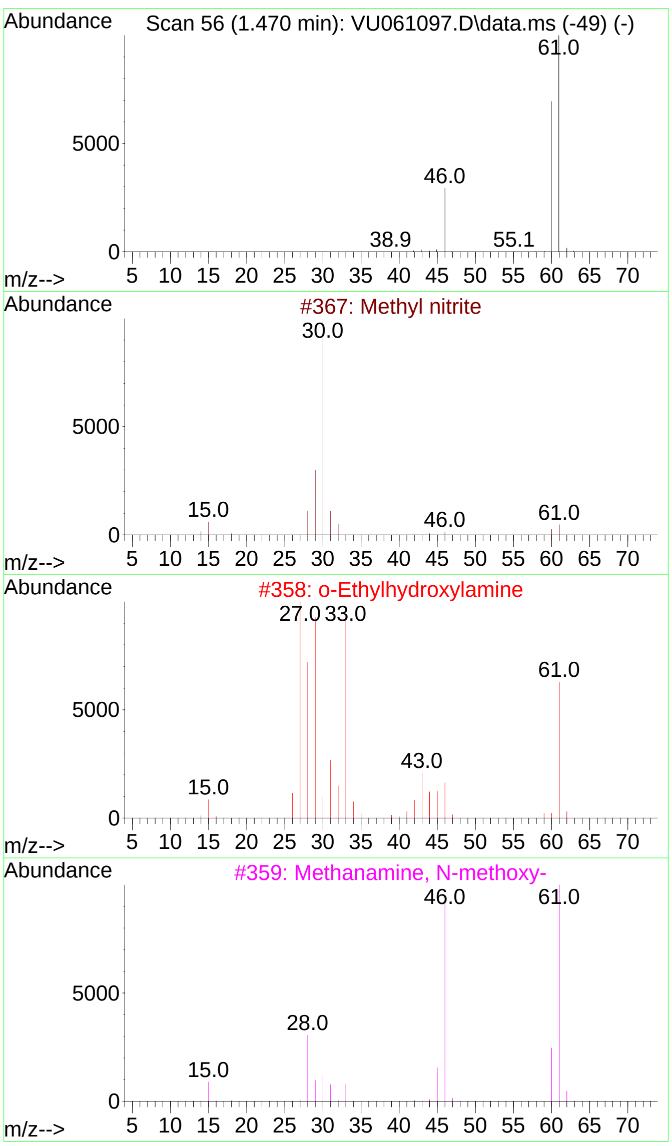
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

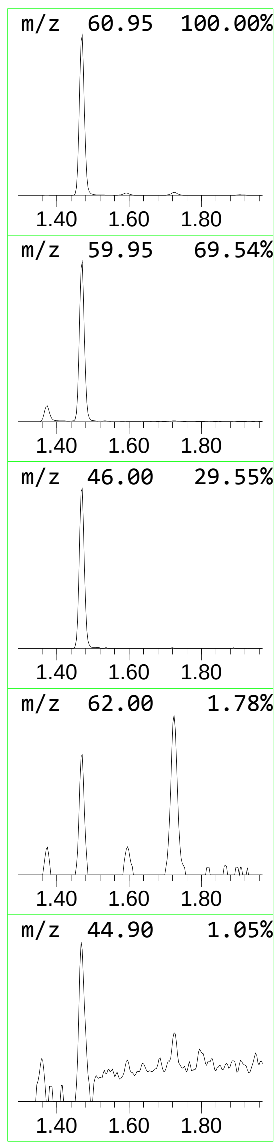
****

Peak Number 2 unknown-02 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.470	2.57 ug/L	209387	1,4-Difluorobenzene	6.242

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methyl nitrite	61	CH3NO2	000624-91-9	5
2	o-Ethylhydroxylamine	61	C2H7NO	000624-86-2	4
3	Methanamine, N-methoxy-	61	C2H7NO	001117-97-1	4
4	Cyanogen chloride	61	CClN	000506-77-4	4
5	Cyanogen chloride	61	CClN	000506-77-4	4





Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

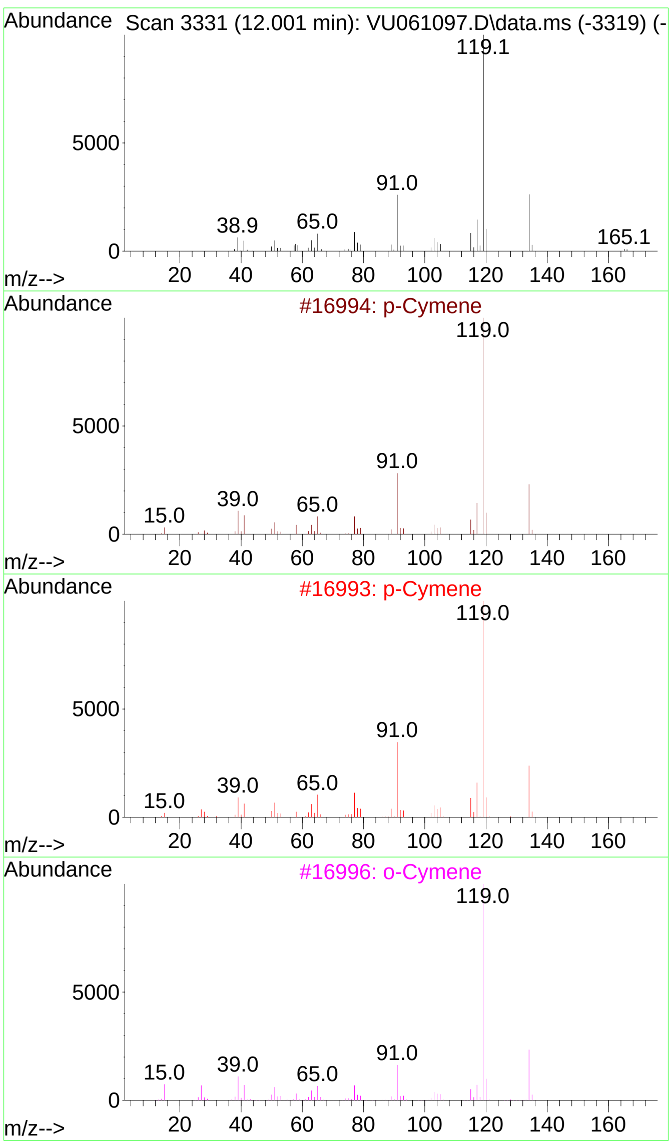
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

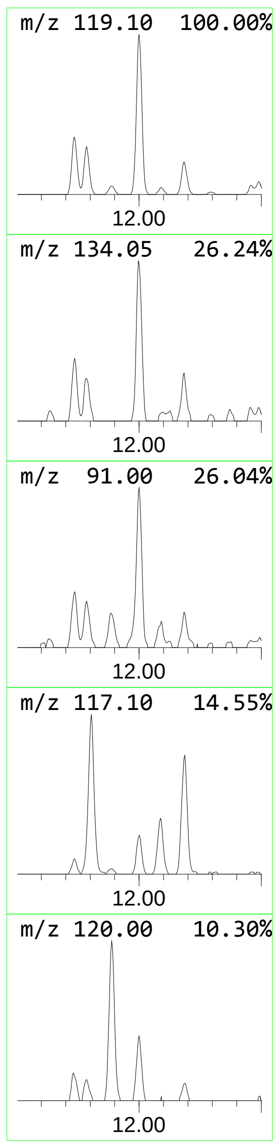
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 p-Cymene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.001	0.71 ug/L	73069	1,4-Dichlorobenzene-d4	11.804

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	p-Cymene	134	C10H14	000099-87-6	97
2	p-Cymene	134	C10H14	000099-87-6	95
3	o-Cymene	134	C10H14	000527-84-4	94
4	o-Cymene	134	C10H14	000527-84-4	94
5	p-Cymene	134	C10H14	000099-87-6	94





Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

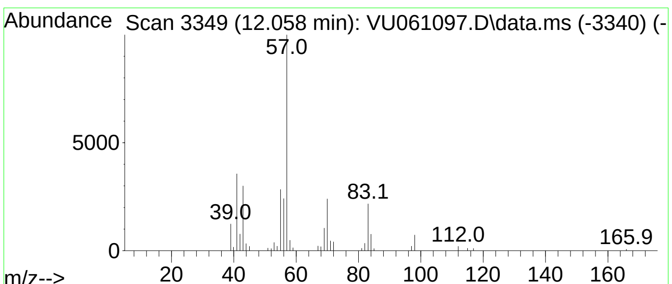
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

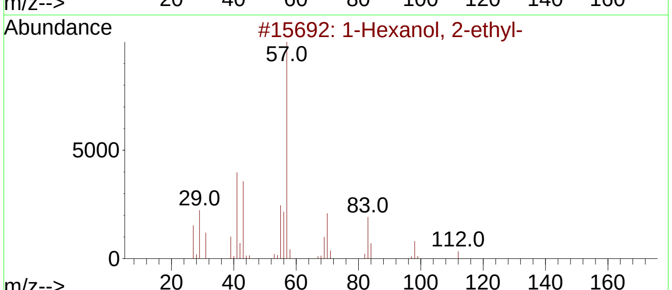
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

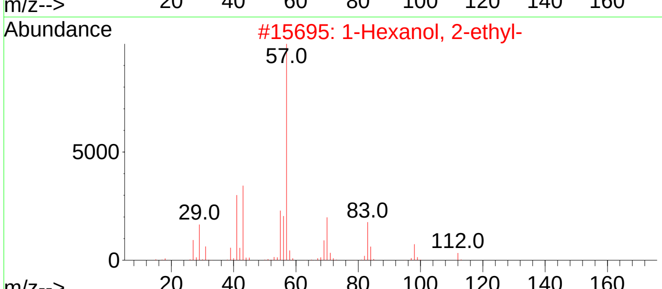
****
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 6

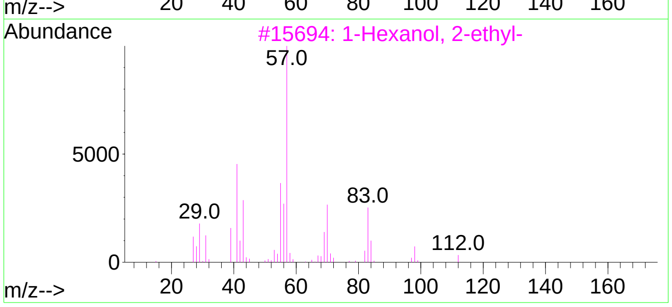
R.T.	EstConc	Area	Relative to ISTD	R.T.
12.059	1.02 ug/L	104769	1,4-Dichlorobenzene-d4	11.804

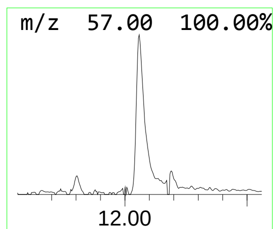
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64

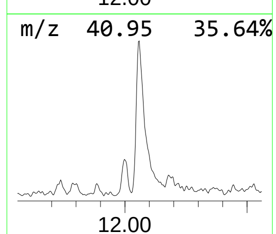


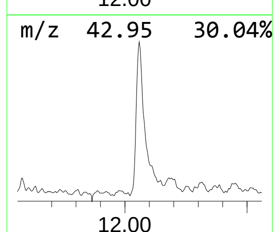


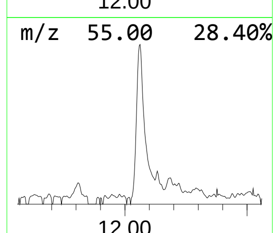


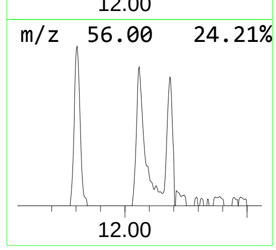












Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

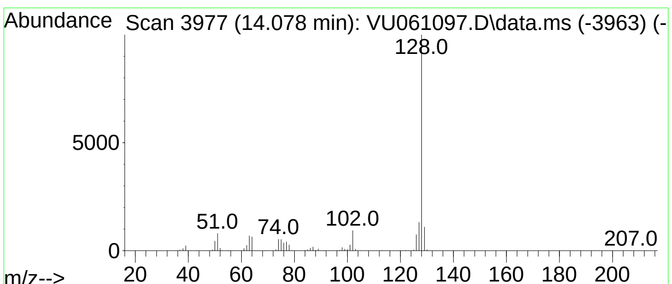
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.M
Quant Title : TRACE VOA SFAM1.0

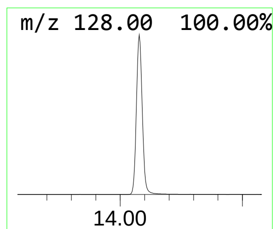
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

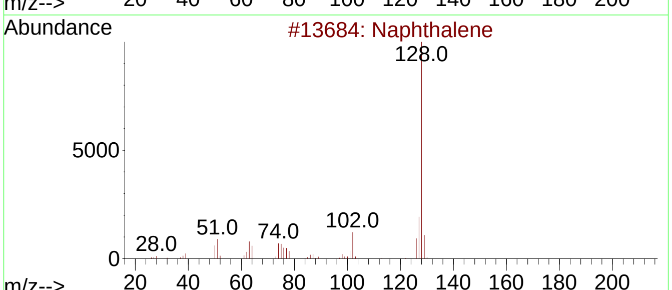
****
Peak Number 7 Azulene Concentration Rank 1

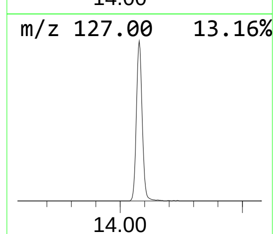
R.T.	EstConc	Area	Relative to ISTD	R.T.
14.078	11.21 ug/L	1150350	1,4-Dichlorobenzene-d4	11.804

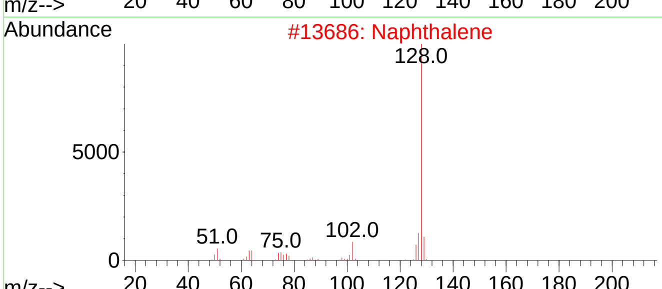
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene	128	C10H8	000091-20-3	97
2	Naphthalene	128	C10H8	000091-20-3	95
3	Naphthalene	128	C10H8	000091-20-3	94
4	Azulene	128	C10H8	000275-51-4	94
5	Naphthalene	128	C10H8	000091-20-3	93

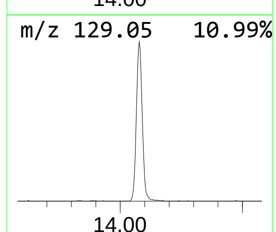


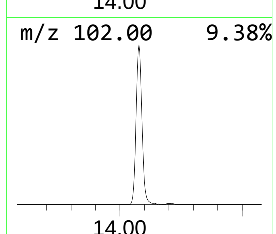


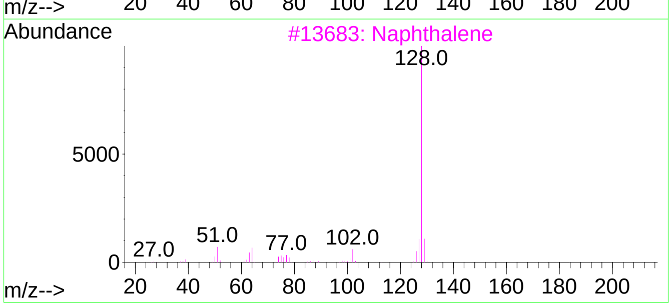


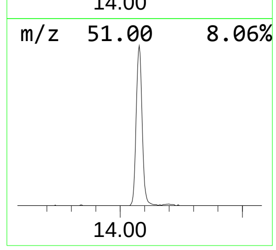












Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101024\
Data File : VU061097.D
Acq On : 10 Oct 2024 18:24
Operator : MD/SY
Sample : P4380-13
Misc : 25.0mL/MSVOA_U/WATER
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
E27H2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMUTR100124WMA.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 #	Internal Standard RT	Internal Standard Resp	Internal Standard Conc
unknown-01	1.358	0.8	ug/L	67951	1	6.242	407554	5.0
unknown-02	1.470	2.6	ug/L	209387	1	6.242	407554	5.0
p-Cymene	12.001	0.7	ug/L	73069	3	11.804	513301	5.0
1-Hexanol, 2-et...	12.059	1.0	ug/L	104769	3	11.804	513301	5.0
Azulene	14.078	11.2	ug/L	1150350	3	11.804	513301	5.0