

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU082321\  
 Data File : VU044510.D  
 Acq On : 23 Aug 2021 19:07  
 Operator : SY/MD  
 Sample : M3517-12  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AG7

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\SFAMUTR081821WMA.M

Title : TRACE VOA SFAM1.0

Signal : TIC: VU044510.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 1.655       | 90            | 98          | 111          | rVB      | 55926          | 66098         | 11.77%          | 1.673%        |
| 2         | 1.977       | 190           | 198         | 209          | rBV      | 50519          | 65094         | 11.59%          | 1.647%        |
| 3         | 2.636       | 392           | 403         | 415          | rBV      | 99249          | 157119        | 27.98%          | 3.976%        |
| 4         | 4.787       | 1039          | 1072        | 1109         | rBV      | 45249          | 215751        | 38.42%          | 5.460%        |
| 5         | 5.179       | 1179          | 1194        | 1212         | rBV      | 86909          | 186380        | 33.19%          | 4.717%        |
| 6         | 5.816       | 1370          | 1392        | 1417         | rBV2     | 176270         | 434437        | 77.36%          | 10.994%       |
| 7         | 6.321       | 1535          | 1549        | 1566         | rBV      | 146308         | 268181        | 47.75%          | 6.787%        |
| 8         | 6.755       | 1669          | 1684        | 1704         | rBV      | 111545         | 212016        | 37.75%          | 5.365%        |
| 9         | 7.610       | 1934          | 1950        | 1967         | rBV      | 49608          | 85921         | 15.30%          | 2.174%        |
| 10        | 7.935       | 2035          | 2051        | 2065         | rBV      | 201129         | 341160        | 60.75%          | 8.633%        |
| 11        | 8.009       | 2065          | 2074        | 2082         | rVB2     | 3445           | 5911          | 1.05%           | 0.150%        |
| 12        | 8.211       | 2126          | 2137        | 2149         | rBV      | 30058          | 48090         | 8.56%           | 1.217%        |
| 13        | 8.664       | 2259          | 2278        | 2313         | rBV      | 299951         | 561609        | 100.00%         | 14.212%       |
| 14        | 8.812       | 2313          | 2324        | 2337         | rBV      | 23216          | 39960         | 7.12%           | 1.011%        |
| 15        | 9.439       | 2506          | 2519        | 2539         | rBV      | 209091         | 342505        | 60.99%          | 8.668%        |
| 16        | 10.095      | 2712          | 2723        | 2737         | rBV      | 8971           | 14574         | 2.60%           | 0.369%        |
| 17        | 10.250      | 2760          | 2771        | 2780         | rBV4     | 5336           | 9232          | 1.64%           | 0.234%        |
| 18        | 10.359      | 2795          | 2805        | 2813         | rVB3     | 5240           | 7744          | 1.38%           | 0.196%        |
| 19        | 10.767      | 2921          | 2932        | 2947         | rVB      | 83969          | 133553        | 23.78%          | 3.380%        |
| 20        | 11.697      | 3212          | 3221        | 3233         | rBV3     | 7463           | 10882         | 1.94%           | 0.275%        |
| 21        | 11.819      | 3247          | 3259        | 3273         | rBB      | 204761         | 322101        | 57.35%          | 8.151%        |
| 22        | 12.066      | 3320          | 3336        | 3362         | rBV      | 42150          | 82986         | 14.78%          | 2.100%        |
| 23        | 12.201      | 3366          | 3378        | 3393         | rVB      | 192065         | 303370        | 54.02%          | 7.677%        |
| 24        | 12.893      | 3585          | 3593        | 3604         | rBV2     | 19765          | 29315         | 5.22%           | 0.742%        |
| 25        | 13.989      | 3925          | 3934        | 3942         | rBV4     | 5601           | 7608          | 1.35%           | 0.193%        |

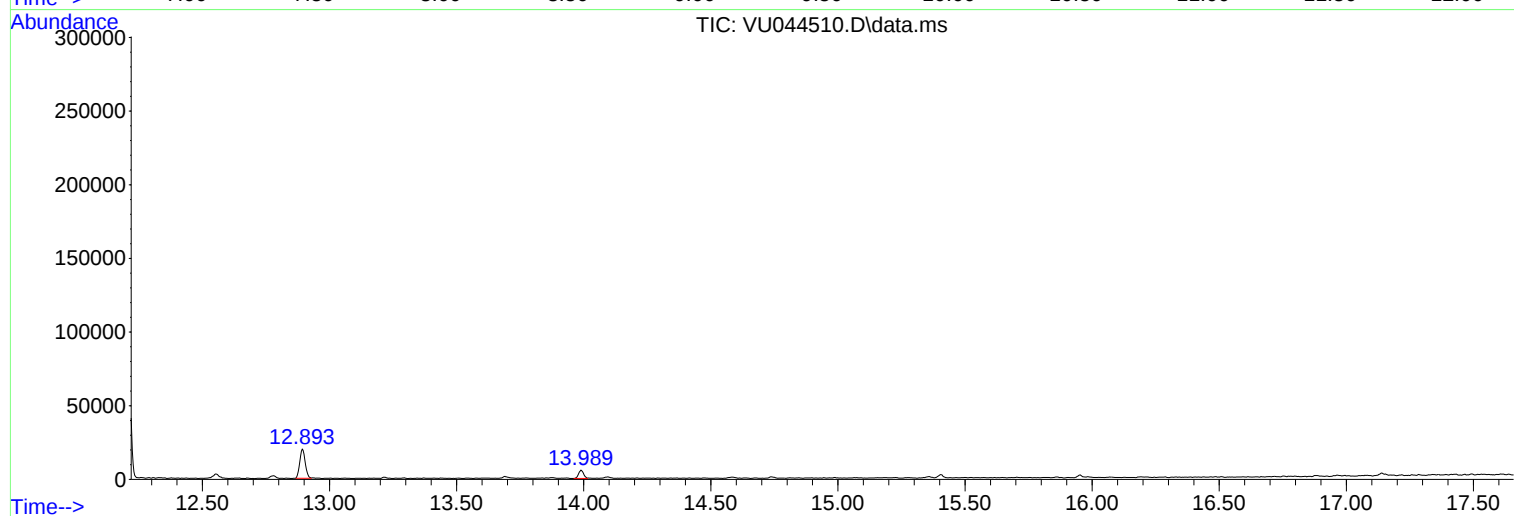
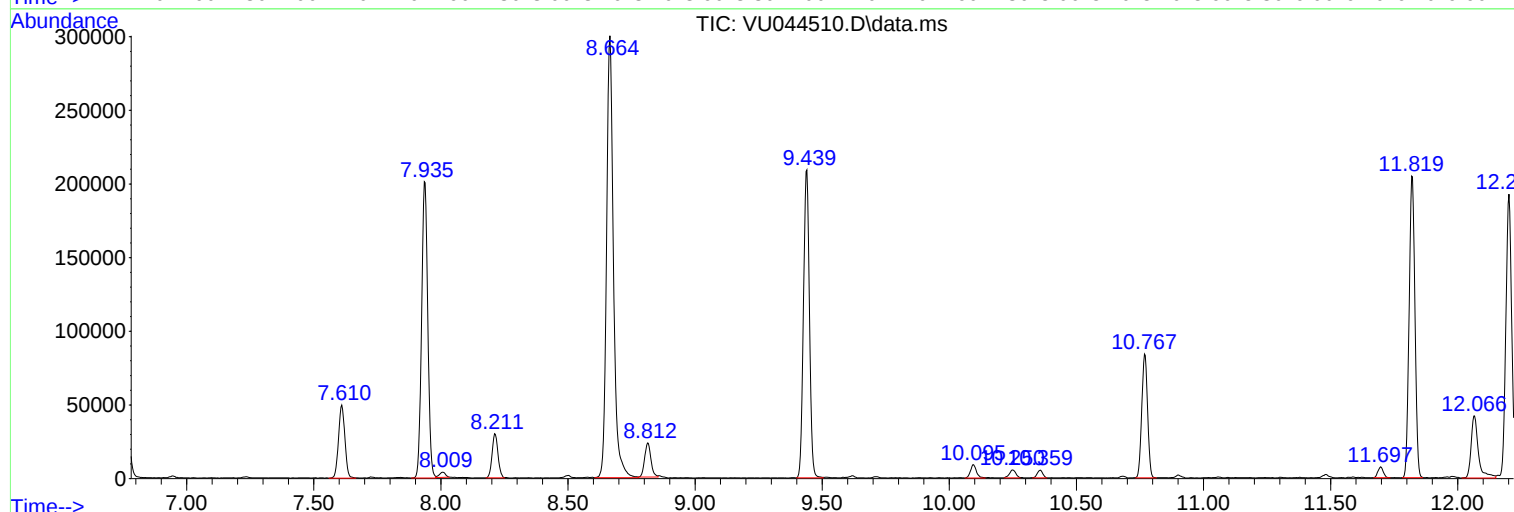
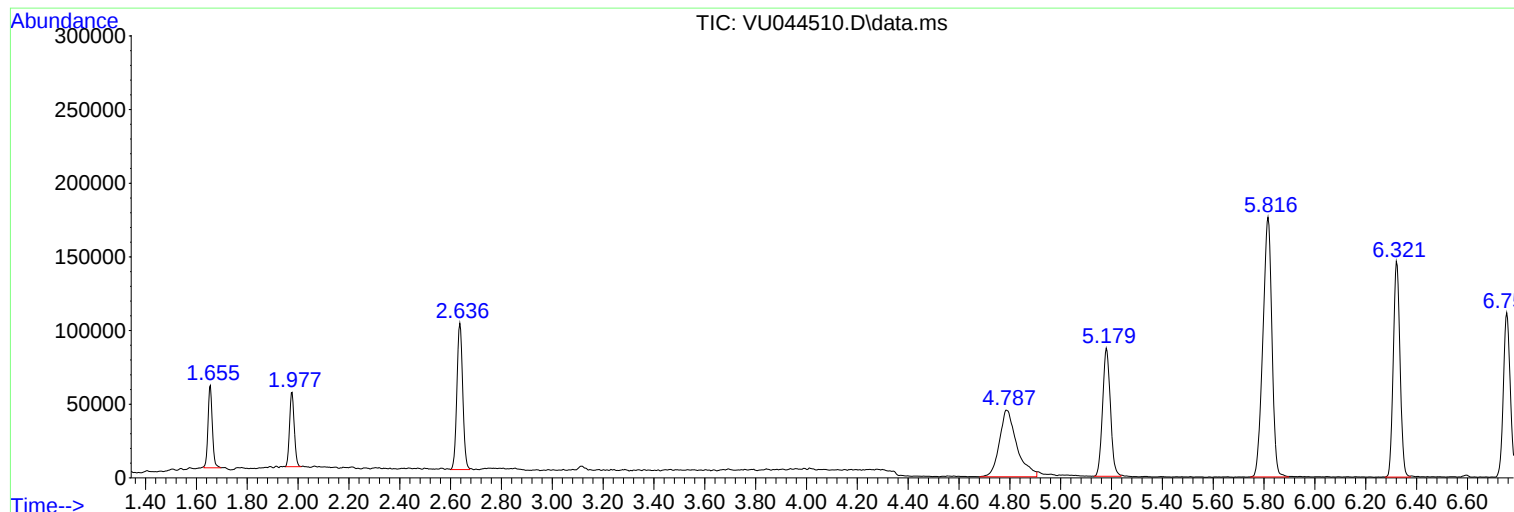
Sum of corrected areas: 3951597

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Instrument :  
MSVOA\_U  
ClientSampleId :  
C0AG7

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR081821WMA.M  
Quant Title : TRACE VOA SFAM1.0

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



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MSVOA\_U  
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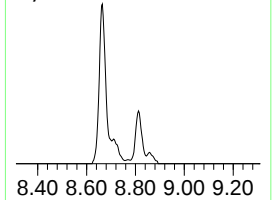
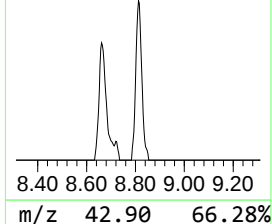
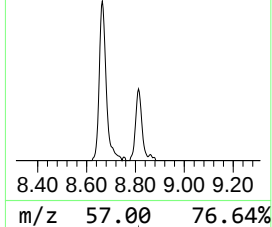
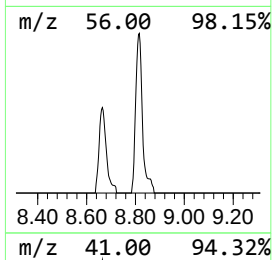
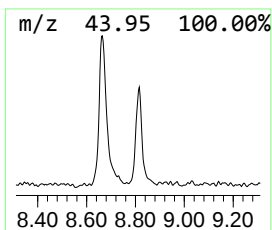
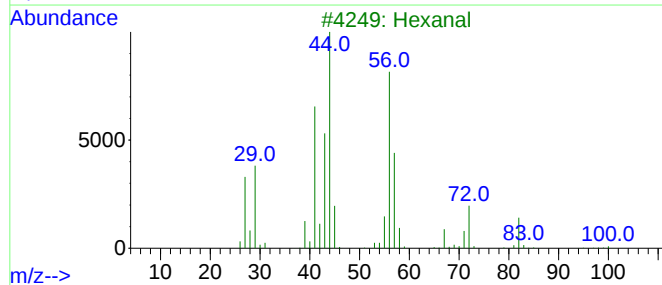
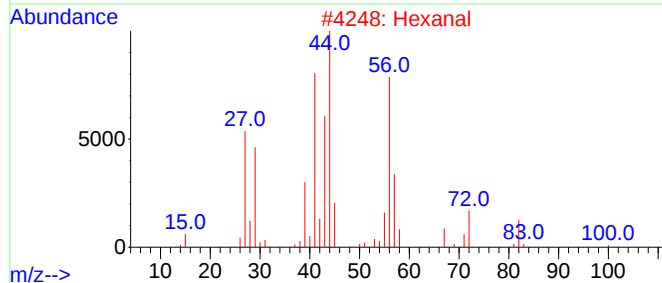
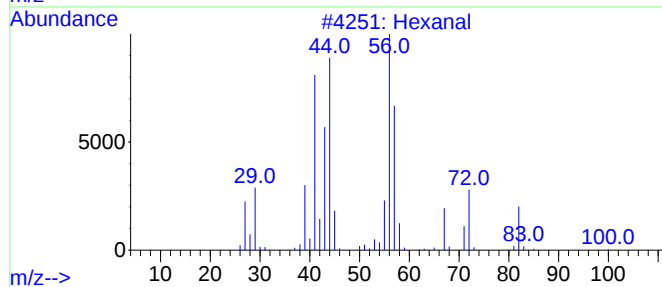
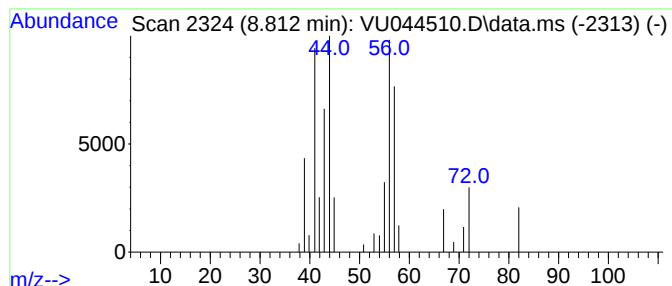
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR081821WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Hexanal Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 8.812 | 0.58 ug/L | 39960 | Chlorobenzene-d5 | 9.439 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal                             |   |              | 100 | C6H12O  | 000066-25-1 | 80   |
| 2    | Hexanal                             |   |              | 100 | C6H12O  | 000066-25-1 | 59   |
| 3    | Hexanal                             |   |              | 100 | C6H12O  | 000066-25-1 | 59   |
| 4    | Hexanal                             |   |              | 100 | C6H12O  | 000066-25-1 | 59   |
| 5    | 2,2-Dimethyl-3-hydroxypropionald... |   |              | 102 | C5H10O2 | 000597-31-9 | 37   |



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C0AG7

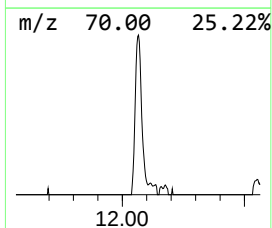
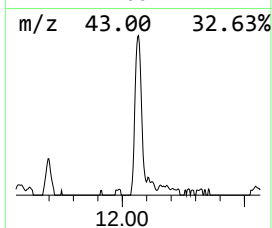
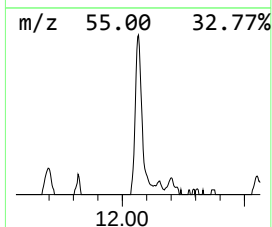
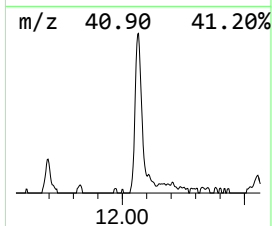
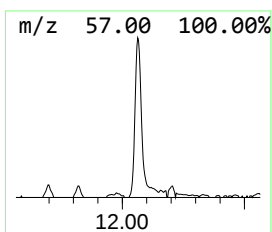
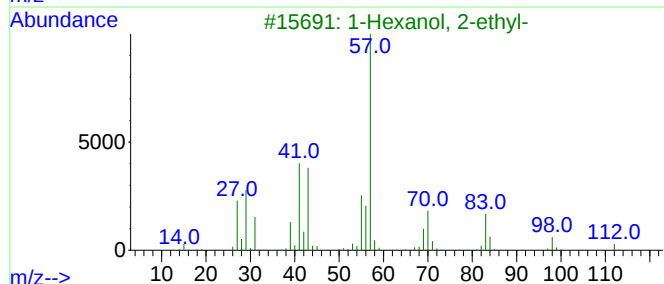
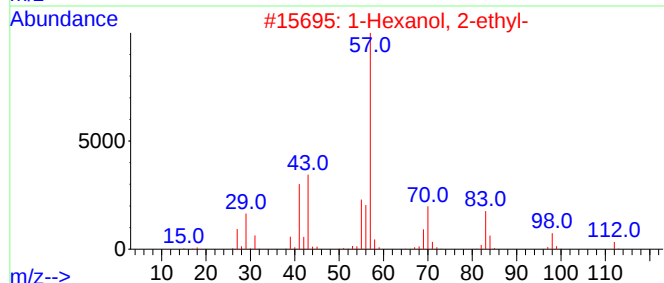
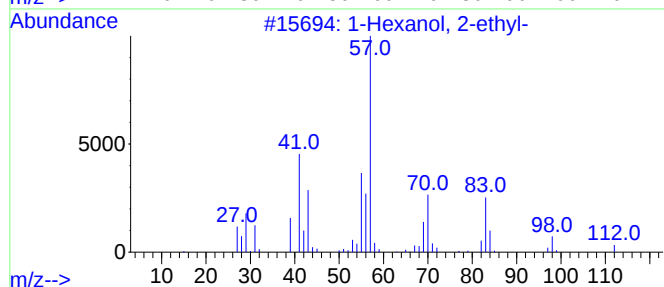
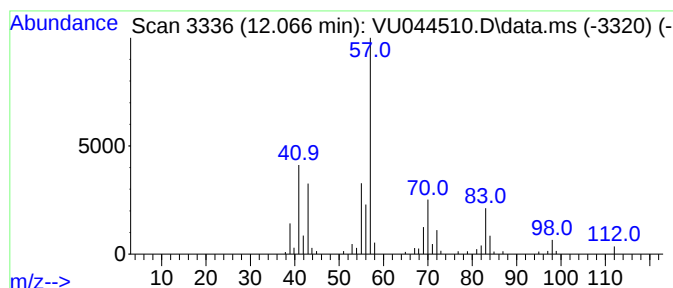
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.066 | 1.29 ug/L | 82986 | 1,4-Dichlorobenzene-d4 | 11.822 |

| Hit# | of                  | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------------------|---|--------------|-----|---------|-------------|------|
| 1    | 1-Hexanol, 2-ethyl- |   |              | 130 | C8H18O  | 000104-76-7 | 86   |
| 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 | 72   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Hexanal            | 8.812  | 0.6     | ug/L  | 39960    | 2                     | 9.439  | 342505 | 5.0  |
| 1-Hexanol, 2-et... | 12.066 | 1.3     | ug/L  | 82986    | 3                     | 11.822 | 322101 | 5.0  |