

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_U\Data\VU082321\  
 Data File : VU044507.D  
 Acq On : 23 Aug 2021 17:54  
 Operator : SY/MD  
 Sample : M3517-05  
 Misc : 25.0mL/MSVOA\_U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 C0AG4

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: VU044507.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         | 1.600       | 73            | 81          | 96           | rBV      | 53087          | 61042         | 11.34%          | 1.623%        |
| 2         | 1.916       | 172           | 179         | 191          | rVB      | 50162          | 64664         | 12.01%          | 1.719%        |
| 3         | 2.571       | 372           | 383         | 400          | rVB      | 90329          | 146791        | 27.27%          | 3.903%        |
| 4         | 4.642       | 1010          | 1027        | 1046         | rBV      | 42432          | 136088        | 25.28%          | 3.618%        |
| 5         | 5.070       | 1145          | 1160        | 1182         | rBV      | 83333          | 184686        | 34.31%          | 4.910%        |
| 6         | 5.732       | 1345          | 1366        | 1390         | rBV2     | 163384         | 435515        | 80.90%          | 11.579%       |
| 7         | 6.256       | 1512          | 1529        | 1546         | rBV      | 147581         | 278795        | 51.79%          | 7.412%        |
| 8         | 6.697       | 1653          | 1666        | 1694         | rBV      | 107560         | 210885        | 39.17%          | 5.607%        |
| 9         | 7.571       | 1925          | 1938        | 1960         | rBV      | 47224          | 86386         | 16.05%          | 2.297%        |
| 10        | 7.906       | 2027          | 2042        | 2059         | rBV      | 195837         | 343575        | 63.82%          | 9.134%        |
| 11        | 7.976       | 2059          | 2064        | 2077         | rVB2     | 4063           | 6115          | 1.14%           | 0.163%        |
| 12        | 8.185       | 2115          | 2129        | 2151         | rBV2     | 28554          | 50886         | 9.45%           | 1.353%        |
| 13        | 8.645       | 2258          | 2272        | 2309         | rBV      | 219384         | 538327        | 100.00%         | 14.312%       |
| 14        | 8.793       | 2309          | 2318        | 2348         | rVB2     | 21259          | 43444         | 8.07%           | 1.155%        |
| 15        | 9.423       | 2500          | 2514        | 2542         | rBV      | 216438         | 363117        | 67.45%          | 9.654%        |
| 16        | 10.089      | 2711          | 2721        | 2743         | rBV2     | 9752           | 18350         | 3.41%           | 0.488%        |
| 17        | 10.243      | 2757          | 2769        | 2788         | rVB3     | 4699           | 9920          | 1.84%           | 0.264%        |
| 18        | 10.761      | 2919          | 2930        | 2947         | rBV      | 82900          | 134155        | 24.92%          | 3.567%        |
| 19        | 11.696      | 3213          | 3221        | 3230         | rVB4     | 4808           | 7183          | 1.33%           | 0.191%        |
| 20        | 11.819      | 3247          | 3259        | 3279         | rVB      | 209069         | 334585        | 62.15%          | 8.895%        |
| 21        | 12.198      | 3361          | 3377        | 3394         | rVB      | 183113         | 293783        | 54.57%          | 7.811%        |
| 22        | 12.896      | 3581          | 3594        | 3608         | rBV3     | 8477           | 13008         | 2.42%           | 0.346%        |

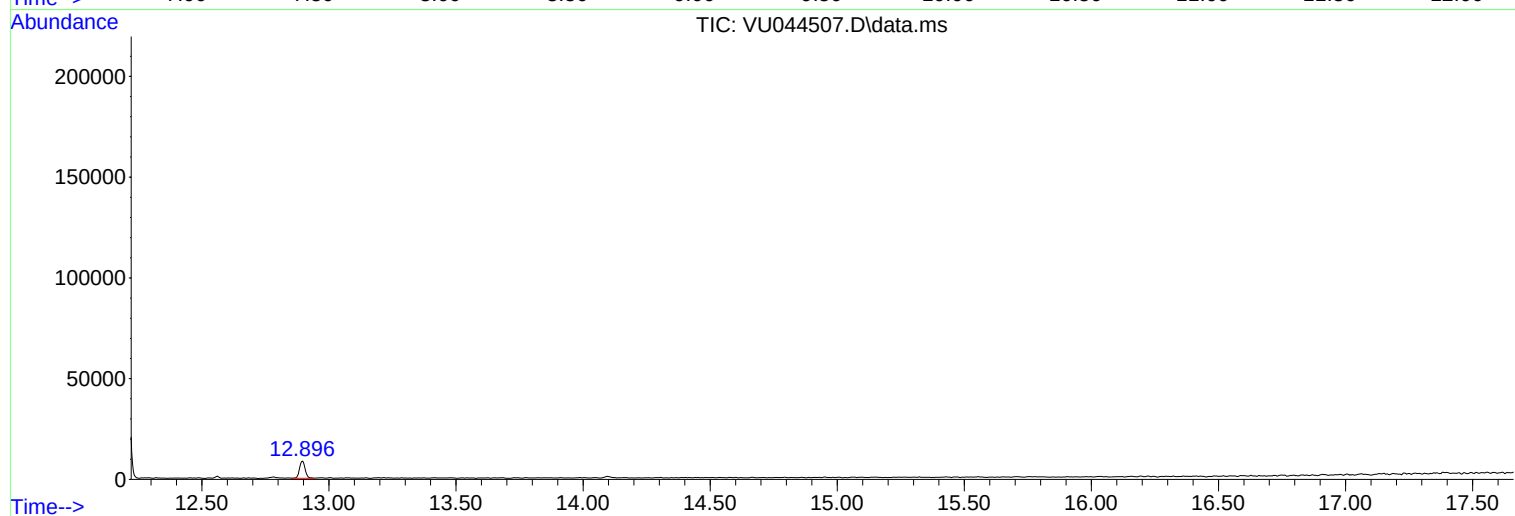
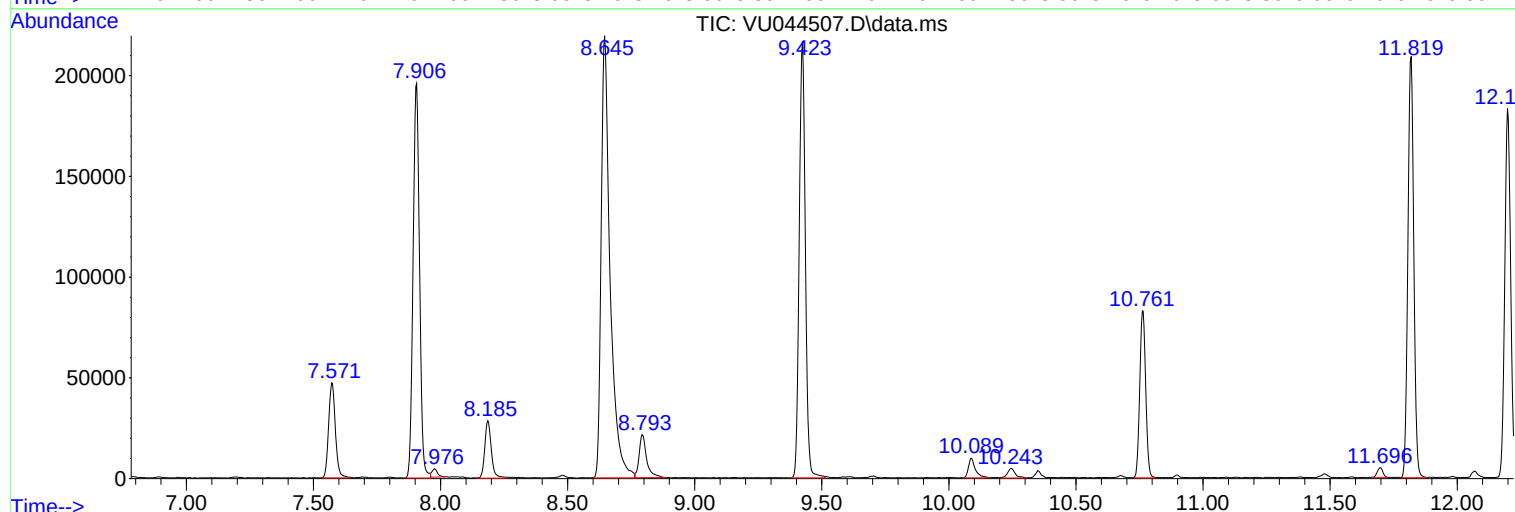
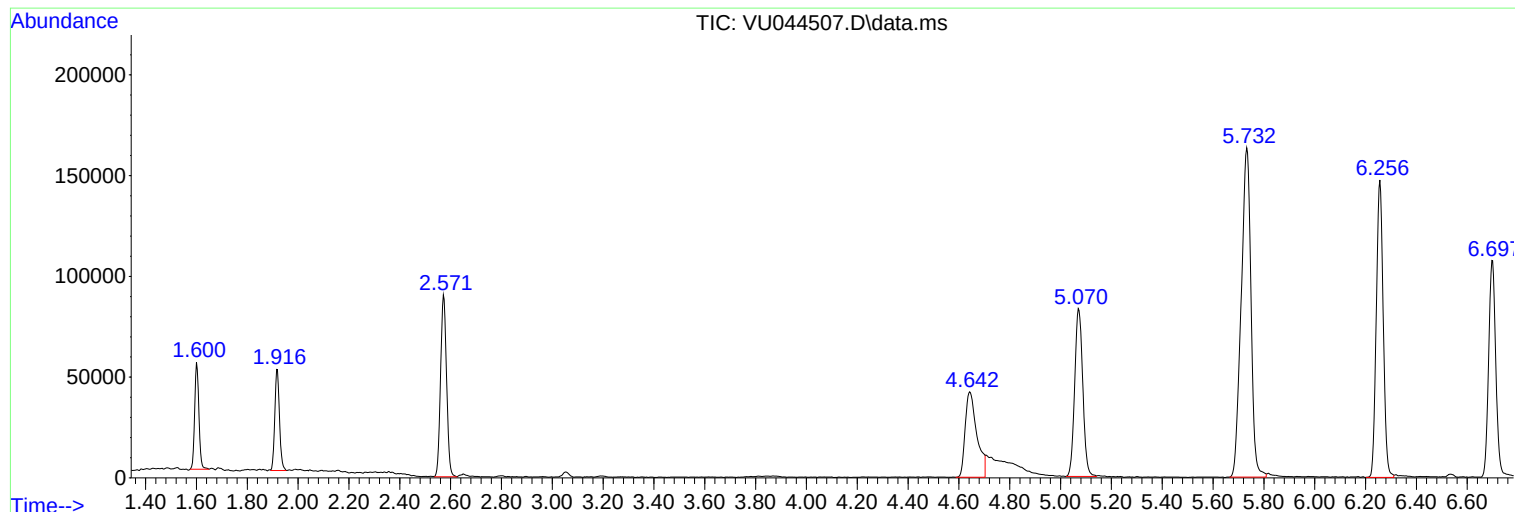
Sum of corrected areas: 3761300

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C0AG4

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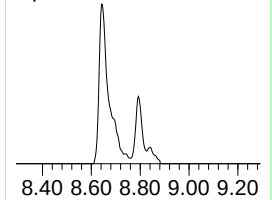
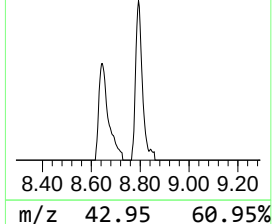
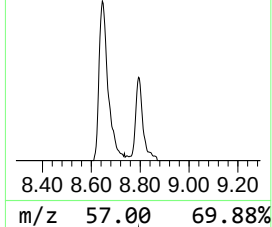
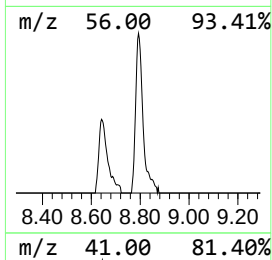
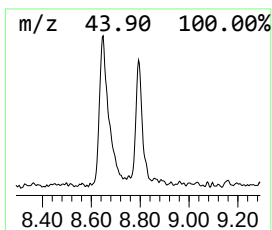
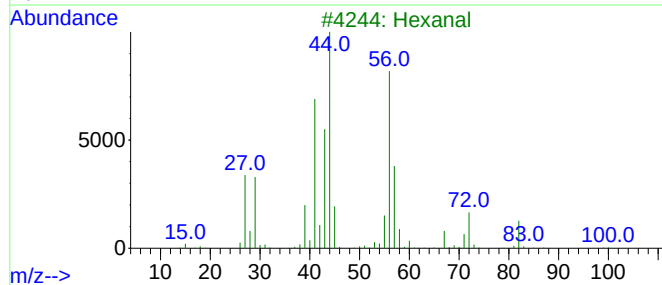
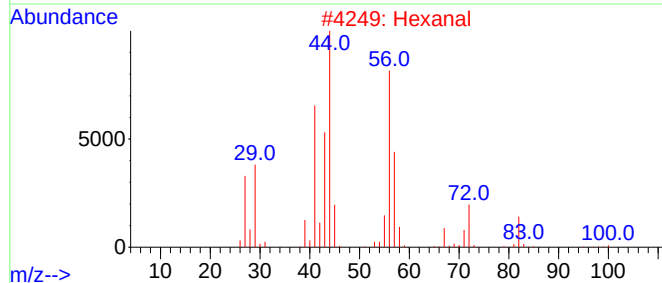
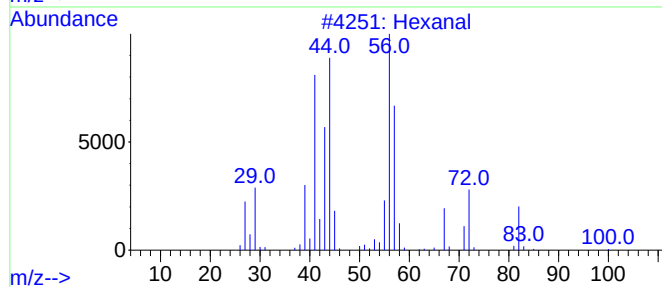
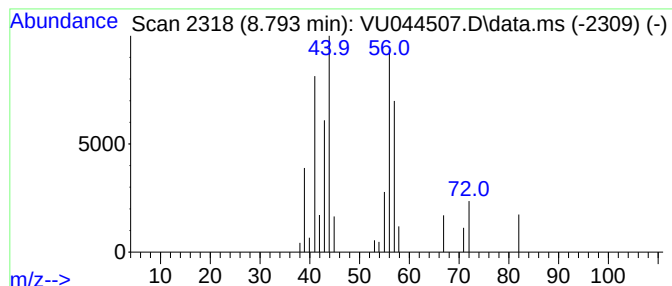
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_U\Method\SFAMUTR081821WMA.M  
Quant Title : TRACE VOA SFAM1.0

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

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Peak Number 2 Hexanal Concentration Rank 2

| R.T.  | EstConc   | Area  | Relative to ISTD | R.T.  |
|-------|-----------|-------|------------------|-------|
| 8.793 | 0.60 ug/L | 43444 | Chlorobenzene-d5 | 9.423 |

| Hit# | of      | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|---------|---|--------------|-----|---------|-------------|------|
| 1    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 80   |
| 2    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 80   |
| 3    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 72   |
| 4    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 64   |
| 5    | Hexanal |   |              | 100 | C6H12O  | 000066-25-1 | 64   |



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| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| Hexanal          | 8.793 | 0.6     | ug/L  | 43444    | 2                     | 9.423 | 363117 | 5.0  |