

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090819\  
 Data File : VU034374.D  
 Acq On : 07 Sep 2019 12:36  
 Operator : JC/SP  
 Sample : K4724-11  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 BFDB1

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.1  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR090119WMA.M  
 Title : TRACE VOA SOM01.0

Signal : TIC

| 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         | 1.396       | 87            | 95          | 105          | rVB      | 124896         | 126426        | 13.77%          | 1.526%        |
| 2         | 1.675       | 174           | 182         | 192          | rBV      | 101869         | 124347        | 13.54%          | 1.501%        |
| 3         | 2.264       | 354           | 365         | 376          | rBV      | 211082         | 318898        | 34.72%          | 3.850%        |
| 4         | 2.312       | 376           | 380         | 390          | rVB      | 11266          | 17099         | 1.86%           | 0.206%        |
| 5         | 2.434       | 410           | 418         | 434          | rVB2     | 19185          | 33262         | 3.62%           | 0.402%        |
| 6         | 4.170       | 945           | 958         | 990          | rBV      | 126025         | 353826        | 38.53%          | 4.272%        |
| 7         | 4.376       | 1011          | 1022        | 1048         | rVB2     | 21728          | 57592         | 6.27%           | 0.695%        |
| 8         | 4.627       | 1082          | 1100        | 1131         | rBV      | 161668         | 394755        | 42.98%          | 4.766%        |
| 9         | 5.318       | 1289          | 1315        | 1351         | rBV2     | 332346         | 918371        | 100.00%         | 11.088%       |
| 10        | 5.865       | 1472          | 1485        | 1512         | rBV      | 347557         | 701956        | 76.43%          | 8.475%        |
| 11        | 6.312       | 1610          | 1624        | 1645         | rBV      | 212511         | 427692        | 46.57%          | 5.164%        |
| 12        | 7.209       | 1892          | 1903        | 1919         | rBV2     | 100759         | 182757        | 19.90%          | 2.207%        |
| 13        | 7.546       | 1995          | 2008        | 2026         | rBV      | 438095         | 770480        | 83.90%          | 9.303%        |
| 14        | 7.833       | 2083          | 2097        | 2118         | rBV2     | 57361          | 108873        | 11.86%          | 1.315%        |
| 15        | 8.296       | 2230          | 2241        | 2277         | rBV      | 416048         | 833757        | 90.79%          | 10.067%       |
| 16        | 8.450       | 2280          | 2289        | 2312         | rVB2     | 60456          | 113254        | 12.33%          | 1.367%        |
| 17        | 9.070       | 2469          | 2482        | 2502         | rBV      | 508794         | 865925        | 94.29%          | 10.455%       |
| 18        | 9.768       | 2689          | 2699        | 2719         | rBV4     | 7198           | 17248         | 1.88%           | 0.208%        |
| 19        | 10.411      | 2887          | 2899        | 2915         | rBV      | 161377         | 267634        | 29.14%          | 3.231%        |
| 20        | 10.591      | 2943          | 2955        | 2968         | rBV3     | 7141           | 12767         | 1.39%           | 0.154%        |
| 21        | 11.463      | 3213          | 3226        | 3250         | rBV      | 540534         | 881075        | 95.94%          | 10.638%       |
| 22        | 11.746      | 3305          | 3314        | 3326         | rBV5     | 6402           | 14150         | 1.54%           | 0.171%        |
| 23        | 11.839      | 3330          | 3343        | 3371         | rVV      | 437783         | 740053        | 80.58%          | 8.935%        |

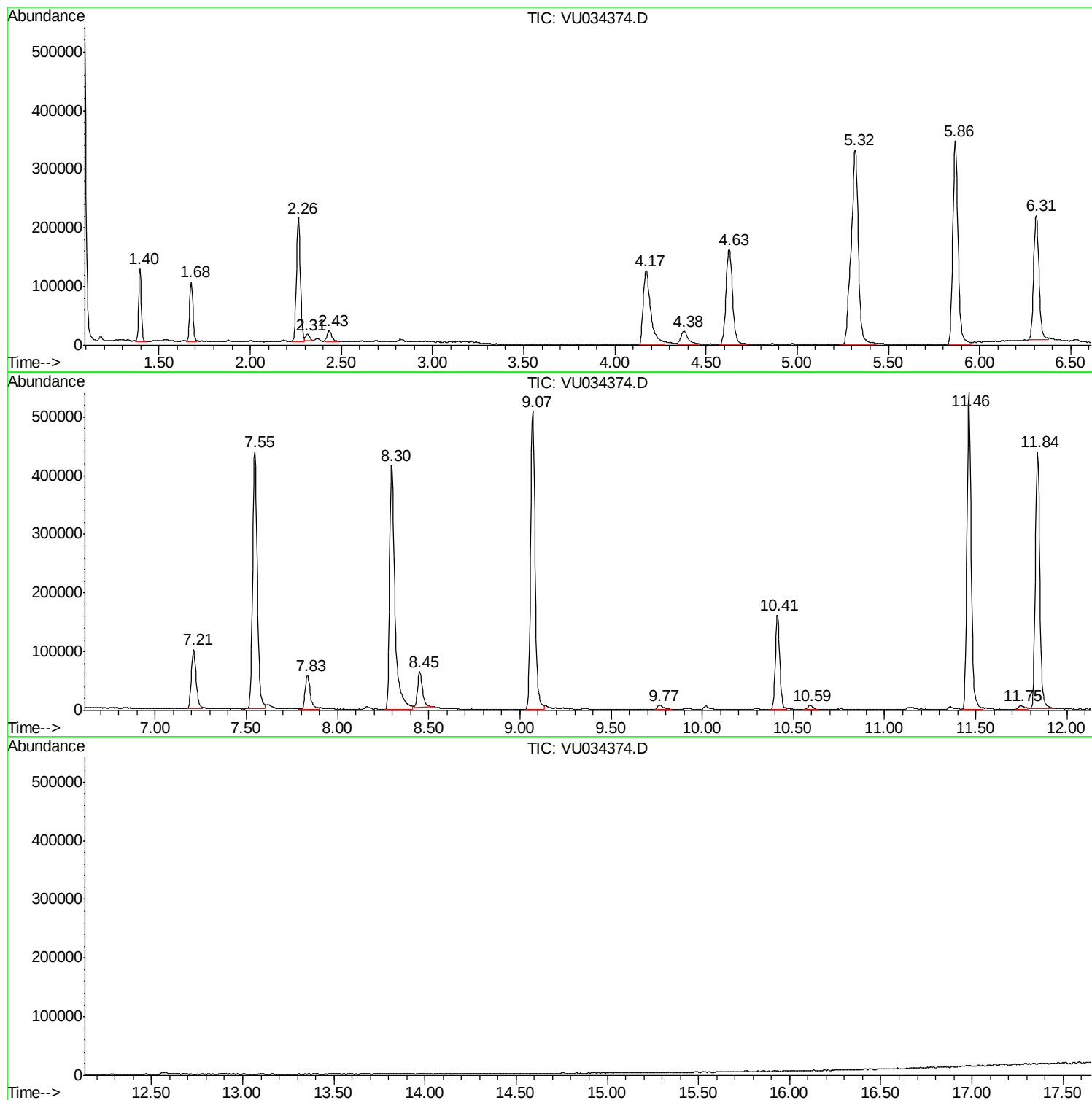
Sum of corrected areas: 8282197

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR090119WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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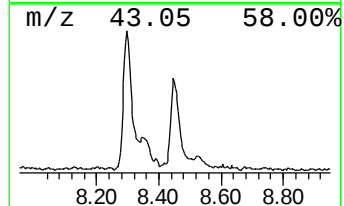
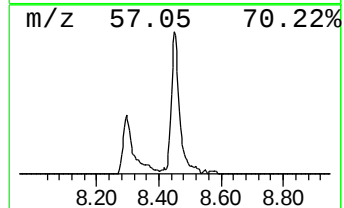
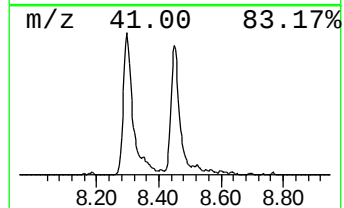
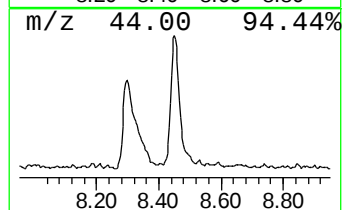
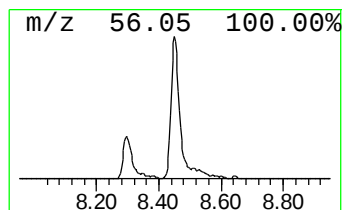
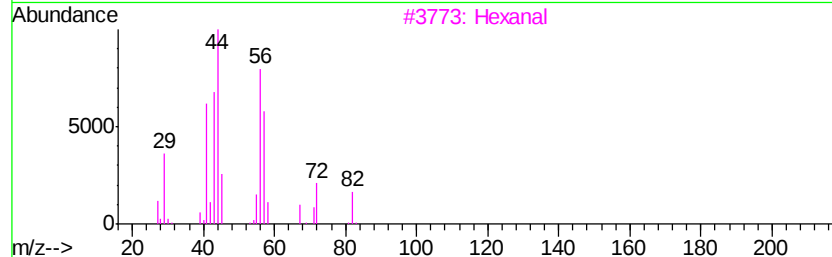
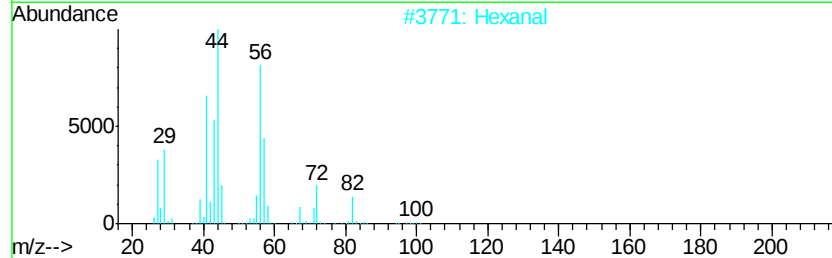
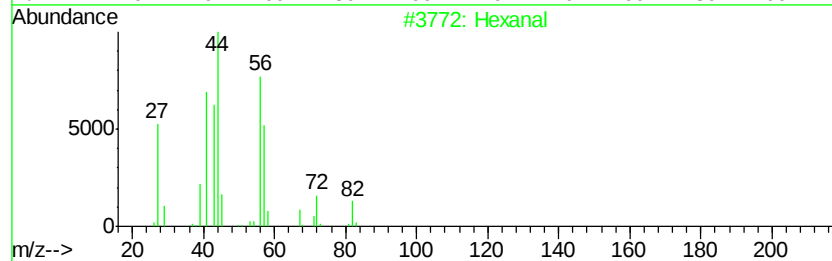
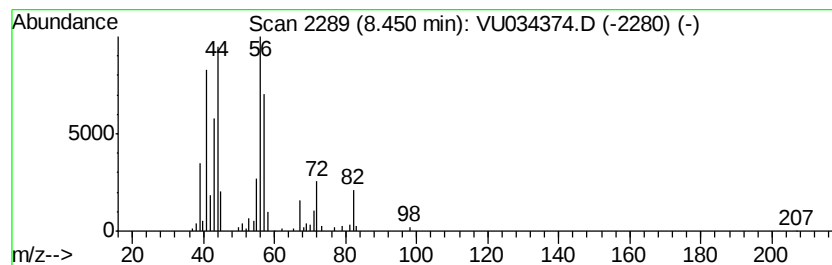
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR090119WMA.M  
Quant Title : TRACE VOA SOM01.0

TIC Library : C:\DATABASE\NIST11.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. |
|------|-----------|--------|------------------|------|
| 8.45 | 0.65 ug/L | 113254 | Chlorobenzene-d5 | 9.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Hexanal                             | 100 | C6H12O  | 000066-25-1 | 90   |
| 2    |    | Hexanal                             | 100 | C6H12O  | 000066-25-1 | 83   |
| 3    |    | Hexanal                             | 100 | C6H12O  | 000066-25-1 | 83   |
| 4    |    | Hexanal                             | 100 | C6H12O  | 000066-25-1 | 83   |
| 5    |    | 2,2-Dimethyl-3-hydroxypropionald... | 102 | C5H10O2 | 000597-31-9 | 32   |



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| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| Hexanal          | 8.45 | 0.7     | ug/L  | 113254   | 2                     | 9.07 | 865925 | 5.0  |