

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100919\  
 Data File : VU035003.D  
 Acq On : 09 Oct 2019 13:14  
 Operator : JC/SP  
 Sample : K5219-12  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 RB-1-190930-01

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\SOMUTR100719WMA.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         | 1.177       | 21            | 27          | 38           | rBV3     | 14316          | 14810         | 2.63%           | 0.294%        |
| 2         | 1.296       | 56            | 64          | 71           | rBV2     | 40807          | 49383         | 8.75%           | 0.982%        |
| 3         | 1.392       | 85            | 94          | 109          | rVB      | 61800          | 70724         | 12.54%          | 1.406%        |
| 4         | 1.470       | 112           | 118         | 126          | rVV2     | 5890           | 7580          | 1.34%           | 0.151%        |
| 5         | 1.672       | 174           | 181         | 193          | rBV      | 56972          | 70527         | 12.50%          | 1.402%        |
| 6         | 2.261       | 354           | 364         | 373          | rBV      | 101164         | 154550        | 27.39%          | 3.072%        |
| 7         | 2.315       | 373           | 381         | 401          | rVB      | 58018          | 101603        | 18.01%          | 2.020%        |
| 8         | 2.441       | 415           | 420         | 432          | rVB2     | 6476           | 11598         | 2.06%           | 0.231%        |
| 9         | 2.685       | 489           | 496         | 507          | rVB3     | 4099           | 7461          | 1.32%           | 0.148%        |
| 10        | 4.170       | 942           | 958         | 992          | rBV      | 80854          | 239424        | 42.44%          | 4.759%        |
| 11        | 4.624       | 1081          | 1099        | 1124         | rBV2     | 85906          | 219869        | 38.97%          | 4.371%        |
| 12        | 5.315       | 1291          | 1314        | 1345         | rBV2     | 177604         | 508726        | 90.17%          | 10.113%       |
| 13        | 5.865       | 1472          | 1485        | 1514         | rBV      | 195403         | 398655        | 70.66%          | 7.925%        |
| 14        | 6.309       | 1607          | 1623        | 1647         | rBV      | 121651         | 252952        | 44.83%          | 5.028%        |
| 15        | 6.524       | 1681          | 1690        | 1706         | rBV2     | 11551          | 24607         | 4.36%           | 0.489%        |
| 16        | 7.209       | 1892          | 1903        | 1926         | rBV      | 51142          | 101739        | 18.03%          | 2.022%        |
| 17        | 7.546       | 1995          | 2008        | 2021         | rBV      | 220444         | 396964        | 70.36%          | 7.891%        |
| 18        | 7.620       | 2021          | 2031        | 2047         | rVB2     | 45997          | 87756         | 15.55%          | 1.744%        |
| 19        | 7.836       | 2085          | 2098        | 2120         | rBV2     | 28616          | 56676         | 10.05%          | 1.127%        |
| 20        | 8.251       | 2218          | 2227        | 2232         | rBV4     | 6118           | 9338          | 1.66%           | 0.186%        |
| 21        | 8.299       | 2232          | 2242        | 2280         | rVV      | 249138         | 564188        | 100.00%         | 11.215%       |
| 22        | 8.450       | 2281          | 2289        | 2306         | rVB4     | 34795          | 66188         | 11.73%          | 1.316%        |
| 23        | 9.035       | 2461          | 2471        | 2472         | rBV3     | 11714          | 14805         | 2.62%           | 0.294%        |
| 24        | 9.070       | 2472          | 2482        | 2519         | rVB      | 290435         | 520452        | 92.25%          | 10.346%       |
| 25        | 9.234       | 2525          | 2533        | 2542         | rVB3     | 6988           | 11641         | 2.06%           | 0.231%        |
| 26        | 9.357       | 2561          | 2571        | 2588         | rBV3     | 12522          | 22264         | 3.95%           | 0.443%        |
| 27        | 9.765       | 2686          | 2698        | 2712         | rBV6     | 12224          | 25410         | 4.50%           | 0.505%        |
| 28        | 10.019      | 2765          | 2777        | 2797         | rBV5     | 8239           | 19308         | 3.42%           | 0.384%        |
| 29        | 10.299      | 2856          | 2864        | 2875         | rBV6     | 5909           | 10486         | 1.86%           | 0.208%        |
| 30        | 10.411      | 2886          | 2899        | 2922         | rBV      | 101334         | 175306        | 31.07%          | 3.485%        |
| 31        | 11.466      | 3215          | 3227        | 3251         | rBV      | 231203         | 442390        | 78.41%          | 8.794%        |
| 32        | 11.842      | 3329          | 3344        | 3369         | rBV      | 205657         | 373244        | 66.16%          | 7.419%        |

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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\SOMUTR100719WMA.M  
Title : TRACE VOA SOM01.0

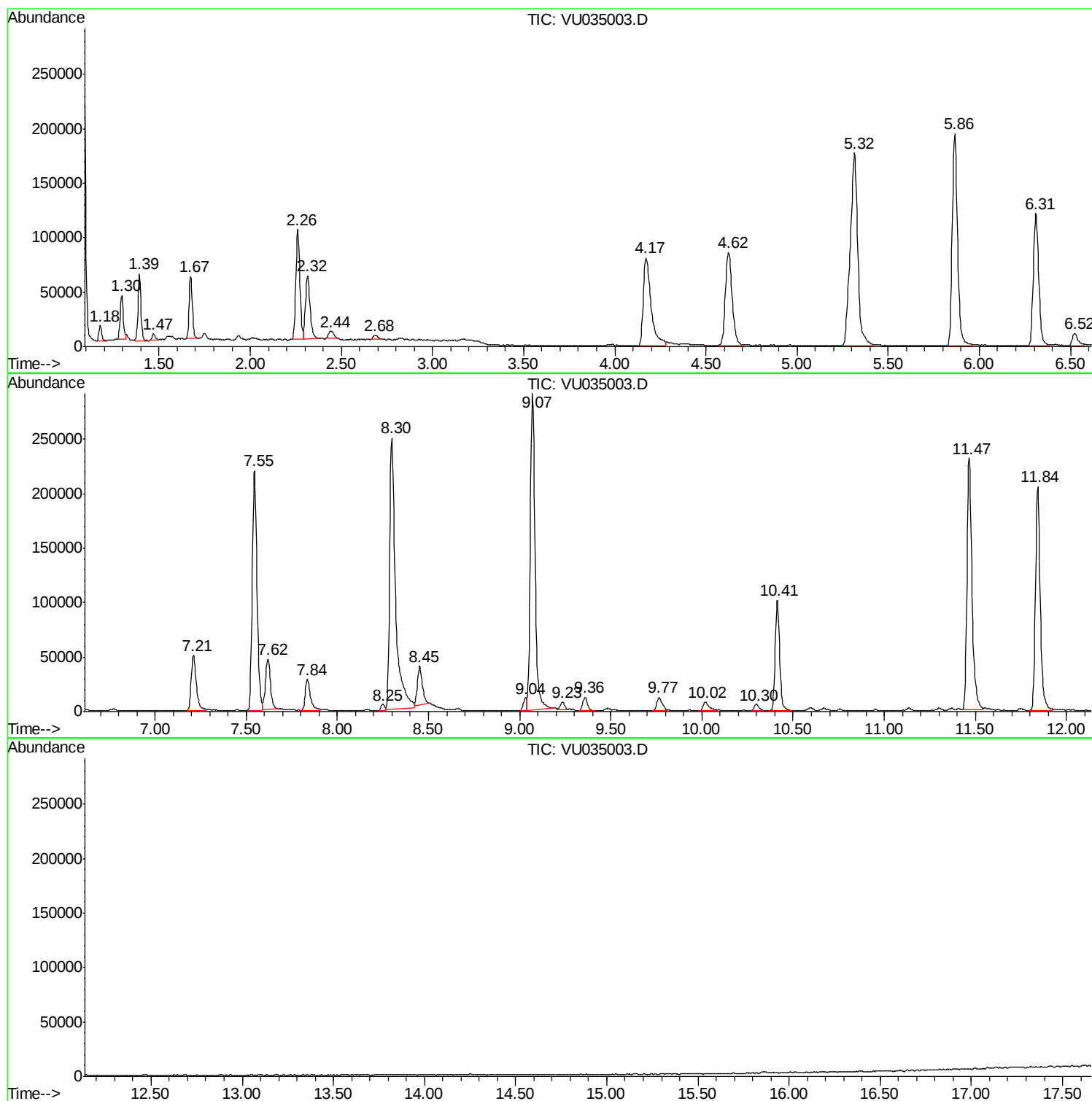
Sum of corrected areas: 5030624

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR100719WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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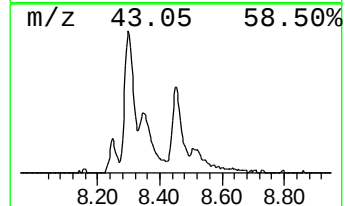
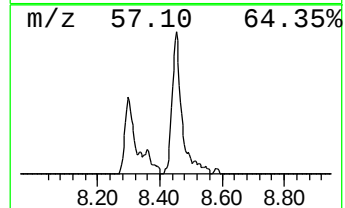
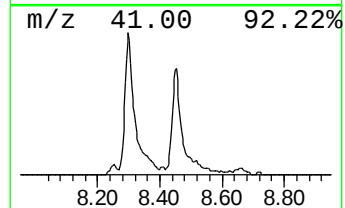
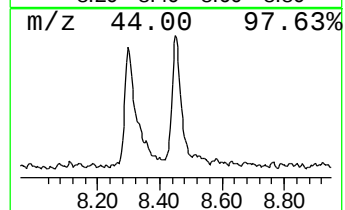
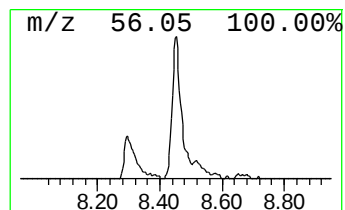
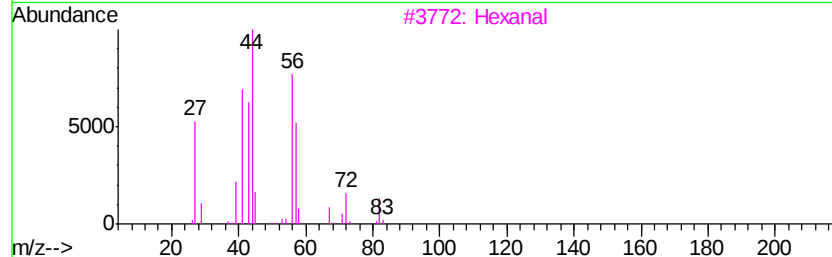
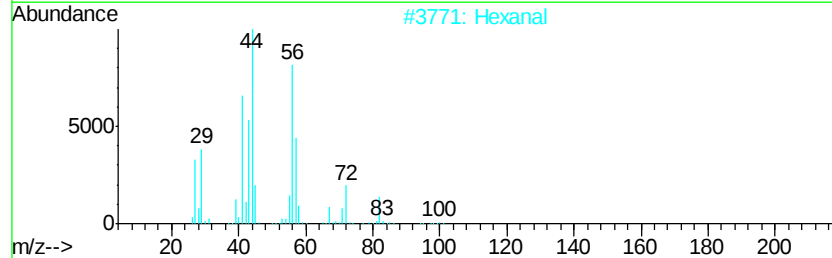
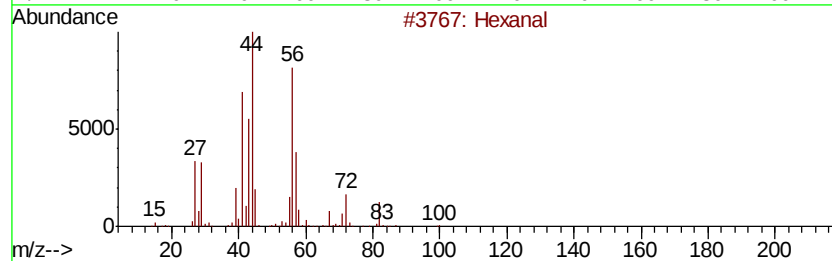
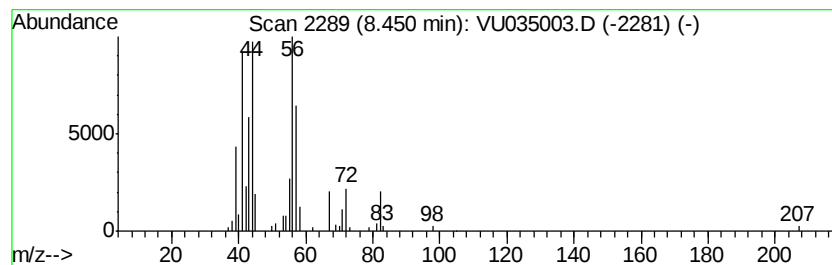
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR100719WMA.M  
Quant Title : TRACE VOA SOM01.0

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 | 0.64 ug/L | 66188 | Chlorobenzene-d5 | 9.07 |

| Hit# | of | Tentative ID     | MW  | MolForm  | CAS#        | Qual |
|------|----|------------------|-----|----------|-------------|------|
| 1    | 5  | Hexanal          | 100 | C6H12O   | 000066-25-1 | 59   |
| 2    |    | Hexanal          | 100 | C6H12O   | 000066-25-1 | 59   |
| 3    |    | Hexanal          | 100 | C6H12O   | 000066-25-1 | 53   |
| 4    |    | Hexanal          | 100 | C6H12O   | 000066-25-1 | 40   |
| 5    |    | Urea, trimethyl- | 102 | C4H10N2O | 000632-14-4 | 35   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                  |      |         |       |          | #                     | RT   | Resp   | Conc |
| Hexanal          | 8.45 | 0.6     | ug/L  | 66188    | 2                     | 9.07 | 520452 | 5.0  |