

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU030119\  
 Data File : VU029769.D  
 Acq On : 01 Mar 2019 17:41  
 Operator : JC/SP  
 Sample : K1660-09  
 Misc : 25.0mL/MSVOA U/WATER  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 MSVOA\_U  
 ClientSampleId :  
 CWK01

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\SOMUTR022119WMA.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         | 1.183       | 23            | 29          | 43           | rBV4     | 12113          | 16409         | 1.14%           | 0.168%        |
| 2         | 1.325       | 67            | 73          | 79           | rBV      | 20349          | 24843         | 1.73%           | 0.254%        |
| 3         | 1.396       | 85            | 95          | 103          | rBV      | 151144         | 189183        | 13.14%          | 1.934%        |
| 4         | 1.679       | 176           | 183         | 197          | rVB      | 102390         | 130040        | 9.03%           | 1.330%        |
| 5         | 2.273       | 358           | 368         | 379          | rBV      | 222380         | 337696        | 23.45%          | 3.453%        |
| 6         | 2.325       | 381           | 384         | 395          | rVB3     | 12233          | 16010         | 1.11%           | 0.164%        |
| 7         | 2.476       | 415           | 431         | 454          | rBV      | 912990         | 1439987       | 100.00%         | 14.724%       |
| 8         | 3.428       | 713           | 727         | 742          | rVB      | 75213          | 160395        | 11.14%          | 1.640%        |
| 9         | 4.219       | 949           | 973         | 1000         | rBV2     | 253194         | 831970        | 57.78%          | 8.507%        |
| 10        | 4.646       | 1089          | 1106        | 1130         | rBV      | 133243         | 319956        | 22.22%          | 3.272%        |
| 11        | 5.334       | 1297          | 1320        | 1350         | rBV2     | 286131         | 777791        | 54.01%          | 7.953%        |
| 12        | 5.884       | 1477          | 1491        | 1513         | rBV      | 260396         | 509038        | 35.35%          | 5.205%        |
| 13        | 6.183       | 1573          | 1584        | 1605         | rBV      | 58539          | 110541        | 7.68%           | 1.130%        |
| 14        | 6.328       | 1615          | 1629        | 1650         | rBV      | 171294         | 346803        | 24.08%          | 3.546%        |
| 15        | 7.225       | 1897          | 1908        | 1932         | rBV      | 89934          | 164855        | 11.45%          | 1.686%        |
| 16        | 7.563       | 1999          | 2013        | 2025         | rBV      | 390305         | 669909        | 46.52%          | 6.850%        |
| 17        | 7.633       | 2025          | 2035        | 2056         | rVB      | 180548         | 327381        | 22.73%          | 3.348%        |
| 18        | 7.849       | 2092          | 2102        | 2118         | rBV2     | 52199          | 91906         | 6.38%           | 0.940%        |
| 19        | 8.173       | 2194          | 2203        | 2217         | rVB      | 11958          | 21145         | 1.47%           | 0.216%        |
| 20        | 8.312       | 2233          | 2246        | 2285         | rBV      | 450520         | 807171        | 56.05%          | 8.254%        |
| 21        | 9.087       | 2475          | 2487        | 2509         | rBV      | 373679         | 630647        | 43.80%          | 6.449%        |
| 22        | 9.373       | 2566          | 2576        | 2586         | rBV2     | 12259          | 19845         | 1.38%           | 0.203%        |
| 23        | 10.431      | 2893          | 2905        | 2927         | rVB2     | 140671         | 228099        | 15.84%          | 2.332%        |
| 24        | 10.604      | 2948          | 2959        | 2971         | rVB      | 20813          | 33364         | 2.32%           | 0.341%        |
| 25        | 11.482      | 3220          | 3232        | 3255         | rBV      | 392799         | 637527        | 44.27%          | 6.519%        |
| 26        | 11.742      | 3301          | 3313        | 3337         | rBV2     | 89806          | 187274        | 13.01%          | 1.915%        |
| 27        | 11.858      | 3337          | 3349        | 3372         | rVB      | 381006         | 637223        | 44.25%          | 6.516%        |
| 28        | 12.469      | 3528          | 3539        | 3554         | rBV4     | 22522          | 50402         | 3.50%           | 0.515%        |
| 29        | 12.582      | 3564          | 3574        | 3589         | rBV4     | 8454           | 18170         | 1.26%           | 0.186%        |
| 30        | 13.832      | 3954          | 3963        | 3979         | rBV2     | 20093          | 44133         | 3.06%           | 0.451%        |

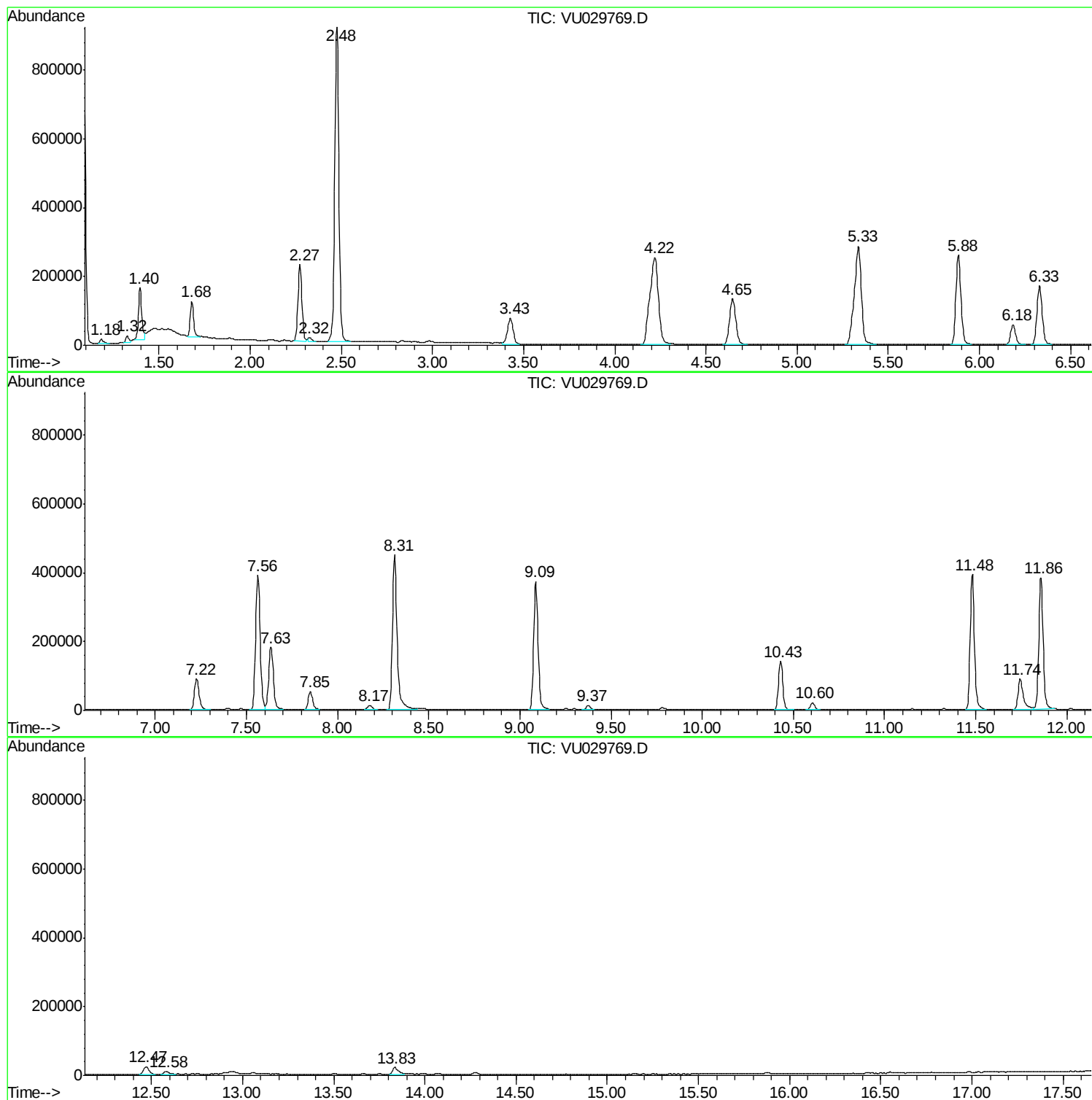
Sum of corrected areas: 9779713

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ClientSampleId :  
CWK01

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_U\METHOD\SOMUTR022119WMA.M  
Quant Title : TRACE VOA SOM01.0

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



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Quant Title : TRACE VOA SOM01.0

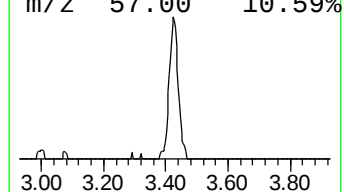
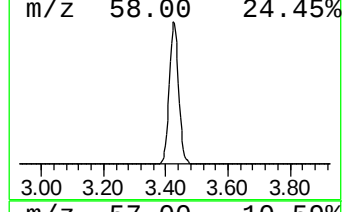
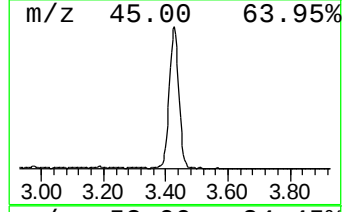
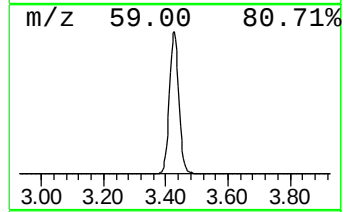
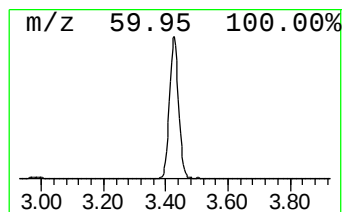
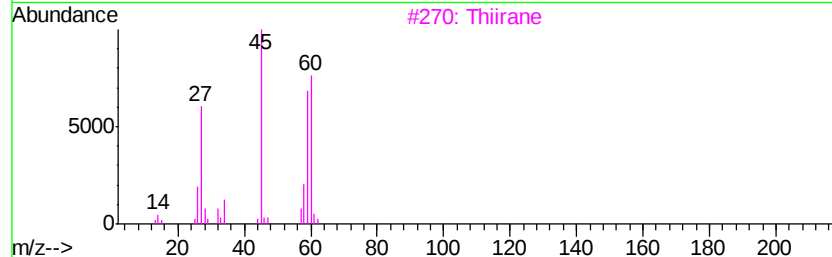
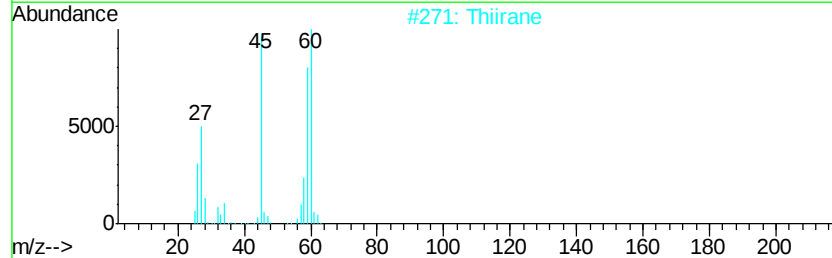
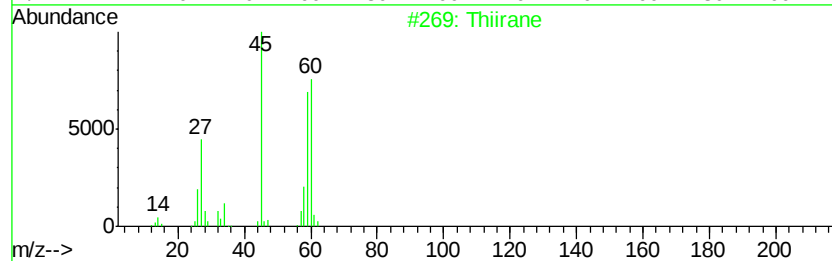
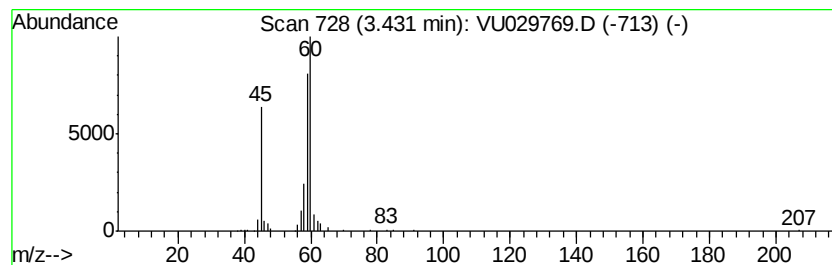
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Thiirane Concentration Rank 2

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 3.43 | 1.58 ug/L | 160395 | 1,4-Difluorobenzene | 5.88 |

| Hit# | of | Tentative ID                    | MW  | MolForm | CAS#        | Qual |
|------|----|---------------------------------|-----|---------|-------------|------|
| 1    | 5  | Thiirane                        | 60  | C2H4S   | 000420-12-2 | 78   |
| 2    |    | Thiirane                        | 60  | C2H4S   | 000420-12-2 | 78   |
| 3    |    | Thiirane                        | 60  | C2H4S   | 000420-12-2 | 64   |
| 4    |    | Thiazole, 4,5-dihydro-2-methyl- | 101 | C4H7NS  | 002346-00-1 | 45   |
| 5    |    | Thiazole, 2-ethyl-4,5-dihydro-  | 115 | C5H9NS  | 016982-46-0 | 40   |



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Instrument :  
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CWK01

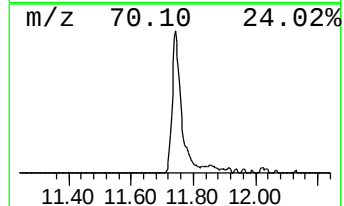
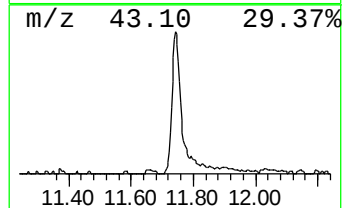
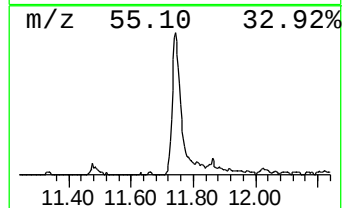
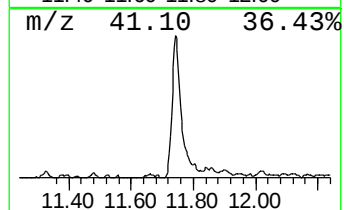
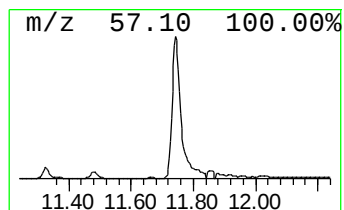
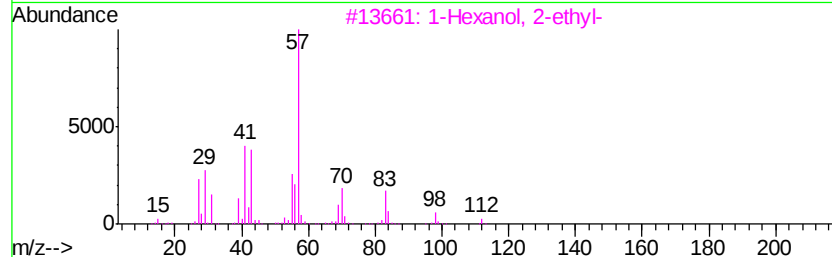
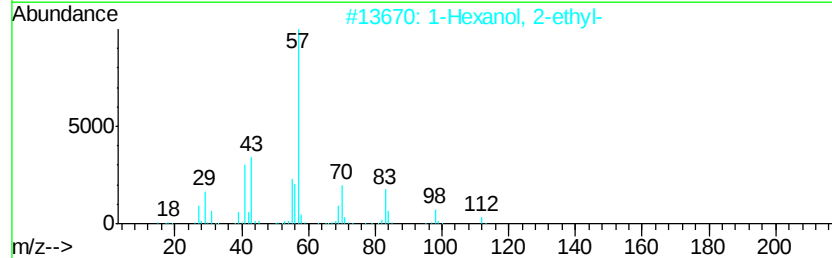
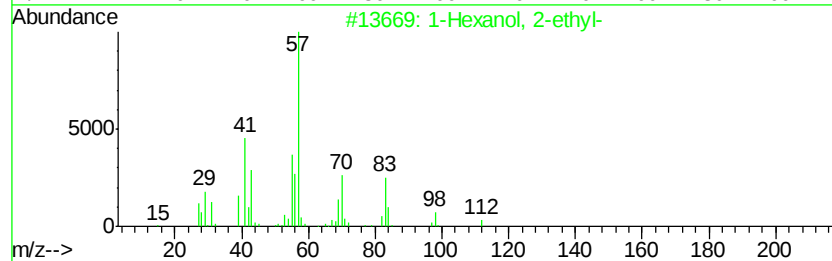
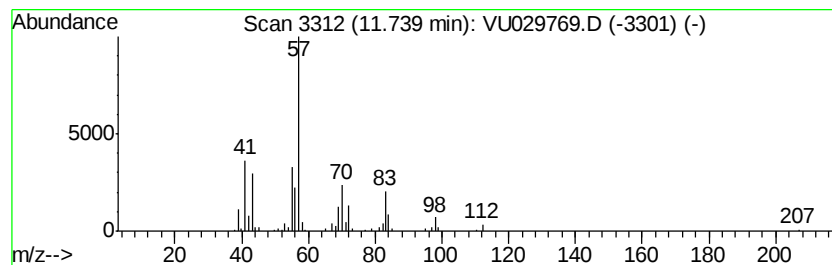
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Quant Title : TRACE VOA SOM01.0

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

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

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 11.74 | 1.47 ug/L | 187274 | 1,4-Dichlorobenzene-d4 | 11.48 |

| 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 | 86   |
| 3    |    |   | 1-Hexanol, 2-ethyl-   | 130 | C8H18O  | 000104-76-7 | 78   |
| 4    |    |   | 1-Hexanol, 2-ethyl-   | 130 | C8H18O  | 000104-76-7 | 59   |
| 5    |    |   | Octane, 2,3-dimethyl- | 142 | C10H22  | 007146-60-3 | 50   |



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| TIC Top Hit name    | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|---------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                     |       |         |       |          | #                     | RT    | Resp   | Conc |
| Thiirane            | 3.43  | 1.6     | ug/L  | 160395   | 1                     | 5.88  | 509038 | 5.0  |
| 1-Hexanol, 2-ethyl- | 11.74 | 1.5     | ug/L  | 187274   | 3                     | 11.48 | 637527 | 5.0  |