

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_N\DATA\VN101618\  
 Data File : VN051895.D  
 Acq On : 16 Oct 2018 14:52  
 Operator : MD\SY  
 Sample : J5527-04  
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 SP-STONE

## Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON Filtering: 5  
 Sampling : 1 Min Area: 3 % of largest Peak  
 Start Thrs: 0.2 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\_N\METHODS\82N101118W.M  
 Title : SW846 8260

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         | 7.593       | 1787          | 1810        | 1821         | rBV      | 604976         | 1507103       | 35.97%          | 7.205%        |
| 2         | 7.667       | 1821          | 1833        | 1866         | rVB      | 959535         | 2290155       | 54.65%          | 10.948%       |
| 3         | 8.027       | 1927          | 1945        | 1970         | rBV2     | 522248         | 1256695       | 29.99%          | 6.008%        |
| 4         | 8.165       | 1973          | 1988        | 2003         | rBV2     | 185602         | 441863        | 10.54%          | 2.112%        |
| 5         | 8.587       | 2103          | 2119        | 2150         | rBV      | 1237940        | 2612073       | 62.34%          | 12.487%       |
| 6         | 9.271       | 2319          | 2332        | 2351         | rBV      | 167449         | 324699        | 7.75%           | 1.552%        |
| 7         | 10.091      | 2571          | 2587        | 2617         | rBV      | 2249081        | 4190311       | 100.00%         | 20.032%       |
| 8         | 10.638      | 2743          | 2757        | 2773         | rBV4     | 28008          | 51643         | 1.23%           | 0.247%        |
| 9         | 10.767      | 2786          | 2797        | 2815         | rBV      | 93700          | 161852        | 3.86%           | 0.774%        |
| 10        | 10.853      | 2816          | 2824        | 2837         | rVB2     | 24481          | 43400         | 1.04%           | 0.207%        |
| 11        | 11.168      | 2904          | 2922        | 2941         | rBV      | 162136         | 276835        | 6.61%           | 1.323%        |
| 12        | 11.410      | 2978          | 2997        | 3022         | rBV      | 1675595        | 3026667       | 72.23%          | 14.469%       |
| 13        | 12.403      | 3291          | 3306        | 3324         | rBV      | 1433972        | 2490355       | 59.43%          | 11.905%       |
| 14        | 13.345      | 3585          | 3599        | 3617         | rVB      | 1335934        | 2244248       | 53.56%          | 10.729%       |

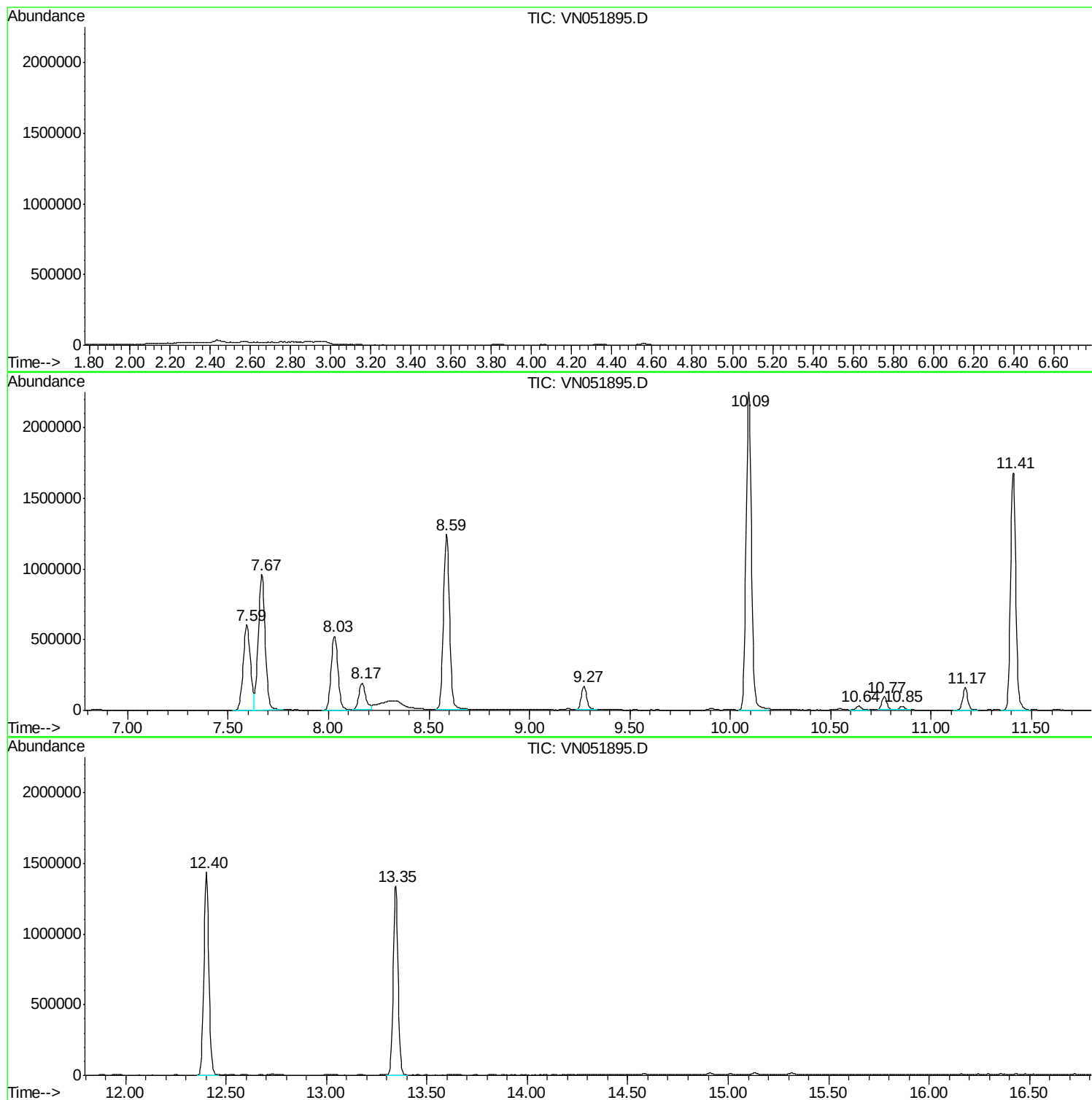
Sum of corrected areas: 20917899

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Instrument :  
MSVOA\_N  
ClientSampleId :  
SP-STONE

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N101118W.M  
Quant Title : SW846 8260

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



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Instrument :  
MSVOA\_N  
ClientSampled :  
SP-STONE

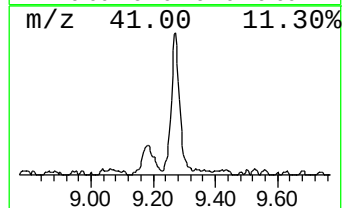
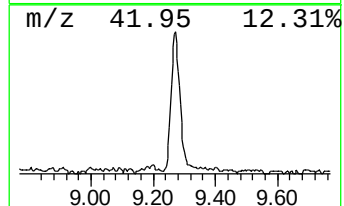
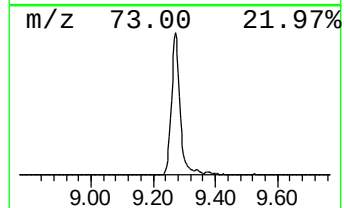
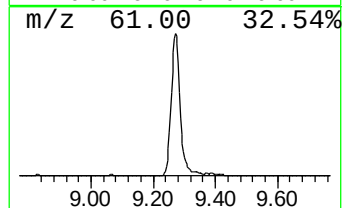
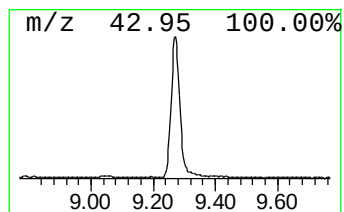
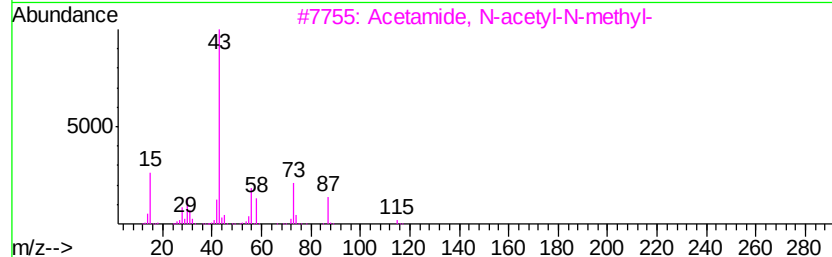
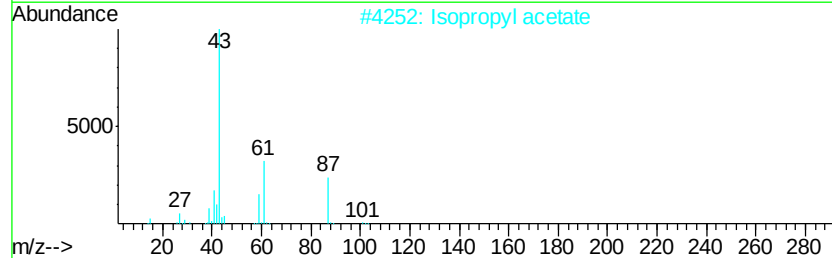
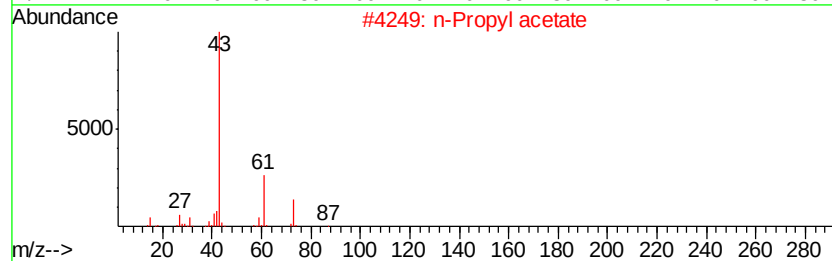
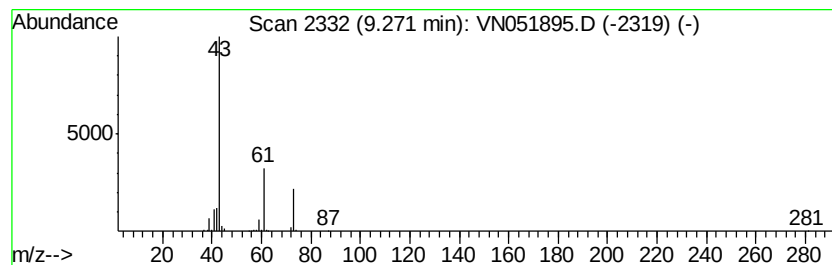
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Quant Title : SW846 8260

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

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Peak Number 1 n-Propyl acetate Concentration Rank 1

| R.T. | EstConc   | Area   | Relative to ISTD    | R.T. |
|------|-----------|--------|---------------------|------|
| 9.27 | 6.22 ug/l | 324699 | 1,4-Difluorobenzene | 8.59 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | n-Propyl acetate               | 102 | C5H10O2 | 000109-60-4 | 74   |
| 2    |    | Isopropyl acetate              | 102 | C5H10O2 | 000108-21-4 | 28   |
| 3    |    | Acetamide, N-acetyl-N-methyl-  | 115 | C5H9NO2 | 001113-68-4 | 9    |
| 4    |    | Isobutyl acetate               | 116 | C6H12O2 | 000110-19-0 | 9    |
| 5    |    | Propanal, 2,3-dihydroxy-, (S)- | 90  | C3H6O3  | 000497-09-6 | 9    |



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| TIC Top Hit name | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                  |      |         |       |          | #                     | RT   | Resp    | Conc |
| n-Propyl acetate | 9.27 | 6.2     | ug/l  | 324699   | 2                     | 8.59 | 2612070 | 50.0 |