

Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_N\DATA\VN032219\  
 Data File : VN054592.D  
 Acq On : 23 Mar 2019 7:50  
 Operator : JC/SP  
 Sample : K2045-18  
 Misc : 5.96g/5mL/100uL/5.00mL/MSVOA\_N/MEOH  
 ALS Vial : 49 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 WP022SB444-190320-(18-20)

## 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\82N032019W.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         | 7.587       | 1792          | 1808        | 1819         | rBV      | 347328         | 857805        | 26.30%          | 5.229%        |
| 2         | 7.661       | 1819          | 1831        | 1853         | rVB      | 648204         | 1539650       | 47.21%          | 9.385%        |
| 3         | 8.024       | 1927          | 1944        | 1963         | rBV      | 426650         | 974993        | 29.90%          | 5.943%        |
| 4         | 8.583       | 2102          | 2118        | 2149         | rBV      | 955942         | 2072645       | 63.56%          | 12.634%       |
| 5         | 10.088      | 2571          | 2586        | 2619         | rBV      | 1463606        | 2905846       | 89.11%          | 17.712%       |
| 6         | 11.406      | 2983          | 2996        | 3034         | rBV2     | 1305536        | 3261044       | 100.00%         | 19.878%       |
| 7         | 12.400      | 3293          | 3305        | 3325         | rBV      | 1037214        | 1766974       | 54.18%          | 10.771%       |
| 8         | 12.963      | 3475          | 3480        | 3492         | rVB3     | 28182          | 43800         | 1.34%           | 0.267%        |
| 9         | 13.088      | 3513          | 3519        | 3529         | rBV4     | 41950          | 68061         | 2.09%           | 0.415%        |
| 10        | 13.342      | 3587          | 3598        | 3620         | rVB      | 1186390        | 2131476       | 65.36%          | 12.992%       |
| 11        | 13.657      | 3687          | 3696        | 3708         | rBV4     | 113095         | 203519        | 6.24%           | 1.241%        |
| 12        | 14.168      | 3848          | 3855        | 3870         | rBV5     | 50139          | 112929        | 3.46%           | 0.688%        |
| 13        | 15.123      | 4146          | 4152        | 4162         | rVB2     | 74800          | 121242        | 3.72%           | 0.739%        |
| 14        | 15.776      | 4350          | 4355        | 4372         | rVB3     | 174356         | 345686        | 10.60%          | 2.107%        |

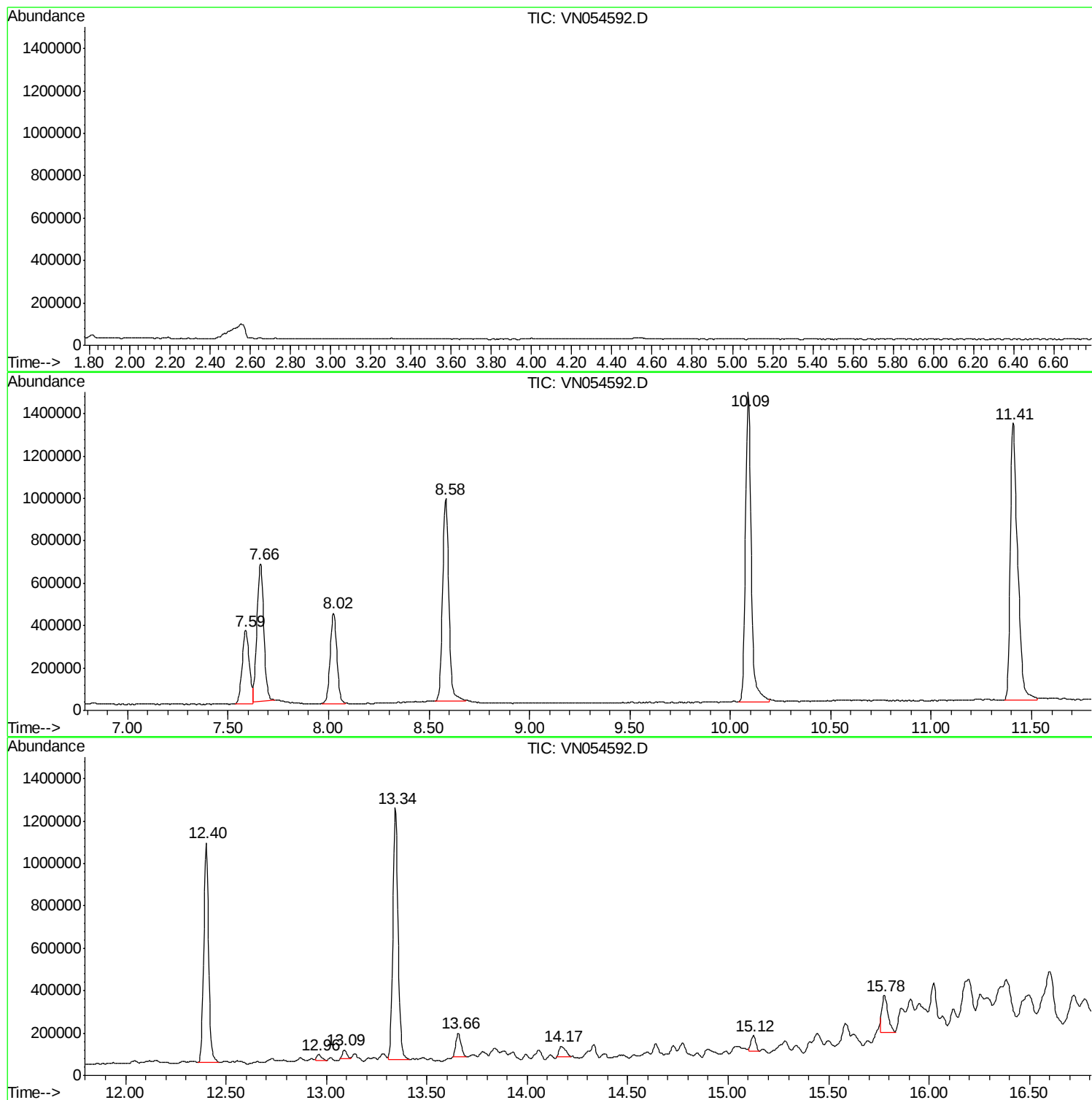
Sum of corrected areas: 16405670

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N032019W.M  
Quant Title : SW846 8260

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



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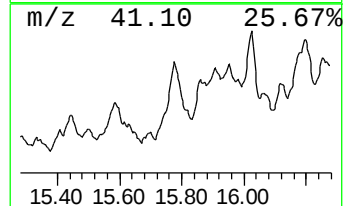
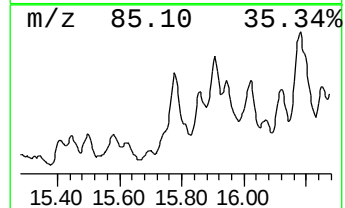
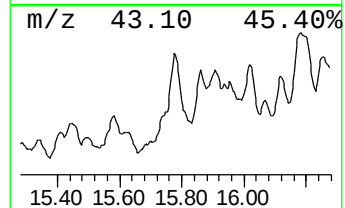
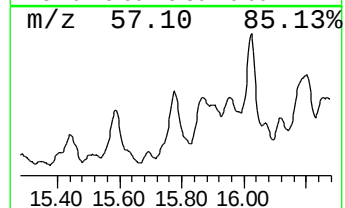
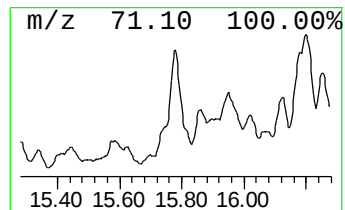
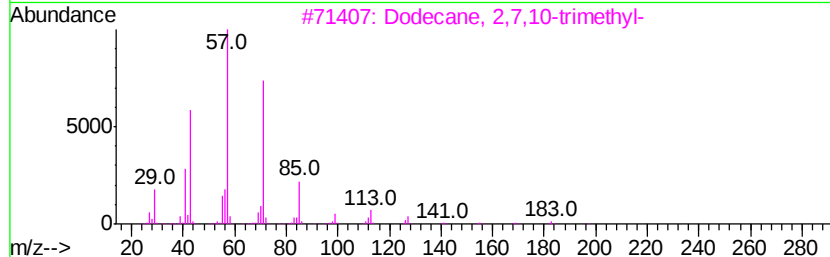
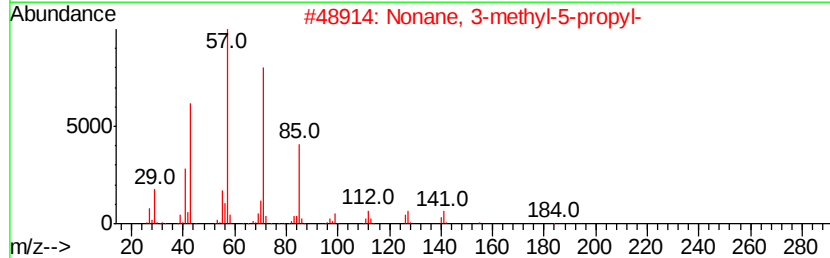
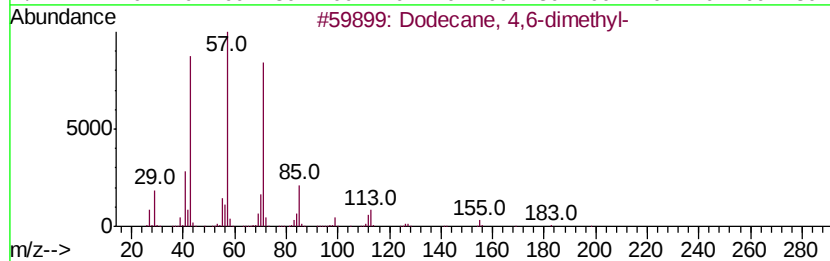
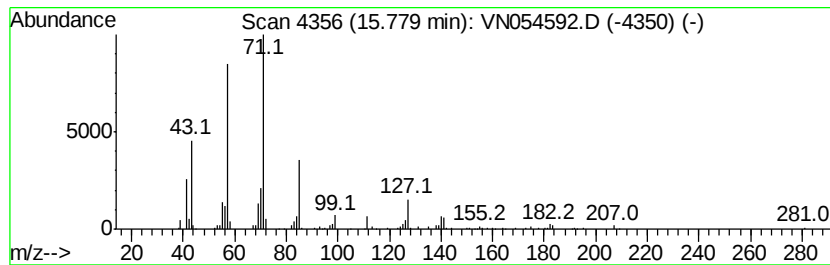
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N032019W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Dodecane, 4,6-dimethyl- Concentration Rank 1

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 15.78 | 8.11 ug/l | 345686 | 1,4-Dichlorobenzene-d4 | 13.34 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Dodecane, 4,6-dimethyl-            | 198 | C14H30  | 061141-72-8 | 72   |
| 2    |    | Nonane, 3-methyl-5-propyl-         | 184 | C13H28  | 031081-18-2 | 72   |
| 3    |    | Dodecane, 2,7,10-trimethyl-        | 212 | C15H32  | 074645-98-0 | 72   |
| 4    |    | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42  | 000638-36-8 | 64   |
| 5    |    | Nonane, 2-methyl-5-propyl-         | 184 | C13H28  | 031081-17-1 | 64   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | # | RT    | Resp    | Conc |
|----------------------|-------|---------|-------|----------|---|-------|---------|------|
| Dodecane, 4,6-dim... | 15.78 | 8.1     | ug/l  | 345686   | 4 | 13.34 | 2131480 | 50.0 |