

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX072020\  
 Data File : VX017436.D  
 Acq On : 20 Jul 2020 16:05  
 Operator : JC/SP  
 Sample : L3329-12  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 ERM-19

Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 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\_X\METHOD\82X071320W.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         | 2.575       | 234           | 244         | 253          | rBV      | 41740          | 81928         | 5.44%           | 0.881%        |
| 2         | 4.653       | 575           | 585         | 594          | rBV      | 12101          | 38745         | 2.57%           | 0.417%        |
| 3         | 5.470       | 707           | 719         | 729          | rBV      | 167043         | 485460        | 32.25%          | 5.221%        |
| 4         | 5.629       | 735           | 745         | 757          | rBV2     | 254798         | 716362        | 47.59%          | 7.704%        |
| 5         | 6.037       | 799           | 812         | 826          | rBV      | 173162         | 464914        | 30.88%          | 5.000%        |
| 6         | 6.830       | 932           | 942         | 961          | rBV      | 423105         | 1014371       | 67.38%          | 10.910%       |
| 7         | 8.695       | 1239          | 1248        | 1258         | rBV      | 913779         | 1408247       | 93.55%          | 15.146%       |
| 8         | 10.098      | 1471          | 1478        | 1494         | rBV      | 998497         | 1345084       | 89.35%          | 14.466%       |
| 9         | 11.122      | 1640          | 1646        | 1658         | rBV      | 911524         | 1132262       | 75.21%          | 12.177%       |
| 10        | 12.061      | 1794          | 1800        | 1806         | rBV      | 1259196        | 1505392       | 100.00%         | 16.190%       |
| 11        | 12.280      | 1829          | 1836        | 1841         | rBV2     | 36571          | 56319         | 3.74%           | 0.606%        |
| 12        | 12.737      | 1907          | 1911        | 1918         | rVB      | 16915          | 23002         | 1.53%           | 0.247%        |
| 13        | 12.878      | 1931          | 1934        | 1940         | rVB      | 16882          | 24190         | 1.61%           | 0.260%        |
| 14        | 12.963      | 1940          | 1948        | 1952         | rBV3     | 13644          | 26384         | 1.75%           | 0.284%        |
| 15        | 13.073      | 1961          | 1966        | 1970         | rBV2     | 12141          | 17295         | 1.15%           | 0.186%        |
| 16        | 13.176      | 1979          | 1983        | 1986         | rBV      | 22605          | 29915         | 1.99%           | 0.322%        |
| 17        | 13.231      | 1986          | 1992        | 1997         | rVB2     | 15569          | 28630         | 1.90%           | 0.308%        |
| 18        | 13.335      | 2005          | 2009        | 2015         | rBV8     | 10012          | 21766         | 1.45%           | 0.234%        |
| 19        | 13.384      | 2015          | 2017        | 2022         | rVB4     | 12068          | 16455         | 1.09%           | 0.177%        |
| 20        | 13.621      | 2052          | 2056        | 2059         | rBV2     | 11194          | 15178         | 1.01%           | 0.163%        |
| 21        | 13.707      | 2068          | 2070        | 2080         | rVB9     | 10661          | 19791         | 1.31%           | 0.213%        |
| 22        | 13.896      | 2097          | 2101        | 2105         | rBV2     | 25305          | 34618         | 2.30%           | 0.372%        |
| 23        | 13.963      | 2105          | 2112        | 2116         | rVV3     | 34722          | 52022         | 3.46%           | 0.559%        |
| 24        | 14.012      | 2116          | 2120        | 2126         | rVB4     | 9651           | 15707         | 1.04%           | 0.169%        |
| 25        | 14.249      | 2155          | 2159        | 2170         | rVB2     | 29591          | 59326         | 3.94%           | 0.638%        |
| 26        | 14.359      | 2172          | 2177        | 2182         | rBV      | 39131          | 52564         | 3.49%           | 0.565%        |
| 27        | 14.420      | 2182          | 2187        | 2191         | rVB2     | 43172          | 65440         | 4.35%           | 0.704%        |
| 28        | 14.530      | 2199          | 2205        | 2208         | rBV2     | 20756          | 34382         | 2.28%           | 0.370%        |
| 29        | 14.639      | 2217          | 2223        | 2228         | rBV      | 47677          | 74442         | 4.95%           | 0.801%        |
| 30        | 14.713      | 2232          | 2235        | 2240         | rVB4     | 11647          | 17505         | 1.16%           | 0.188%        |
| 31        | 14.828      | 2249          | 2254        | 2259         | rBV3     | 28842          | 47301         | 3.14%           | 0.509%        |
| 32        | 15.231      | 2315          | 2320        | 2325         | rVB2     | 23872          | 39455         | 2.62%           | 0.424%        |
| 33        | 15.304      | 2327          | 2332        | 2337         | rBV9     | 10338          | 19417         | 1.29%           | 0.209%        |
| 34        | 15.456      | 2353          | 2357        | 2362         | rVB4     | 16147          | 23372         | 1.55%           | 0.251%        |

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## Integration Parameters: RTEINT.P

Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 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\_X\METHOD\82X071320W.M  
Title : SW846 8260

|    |        |      |      |      |      |       |       |       |        |
|----|--------|------|------|------|------|-------|-------|-------|--------|
| 35 | 15.566 | 2371 | 2375 | 2381 | rVB5 | 15749 | 28240 | 1.88% | 0.304% |
| 36 | 15.664 | 2385 | 2391 | 2395 | rBV5 | 17351 | 28744 | 1.91% | 0.309% |
| 37 | 15.786 | 2405 | 2411 | 2418 | rBV7 | 11926 | 28569 | 1.90% | 0.307% |
| 38 | 15.865 | 2418 | 2424 | 2427 | rVV2 | 34735 | 64600 | 4.29% | 0.695% |
| 39 | 15.901 | 2427 | 2430 | 2438 | rVB  | 34358 | 53657 | 3.56% | 0.577% |
| 40 | 16.048 | 2447 | 2454 | 2465 | rVB  | 29841 | 60380 | 4.01% | 0.649% |
| 41 | 16.389 | 2505 | 2510 | 2515 | rVB2 | 13908 | 26616 | 1.77% | 0.286% |

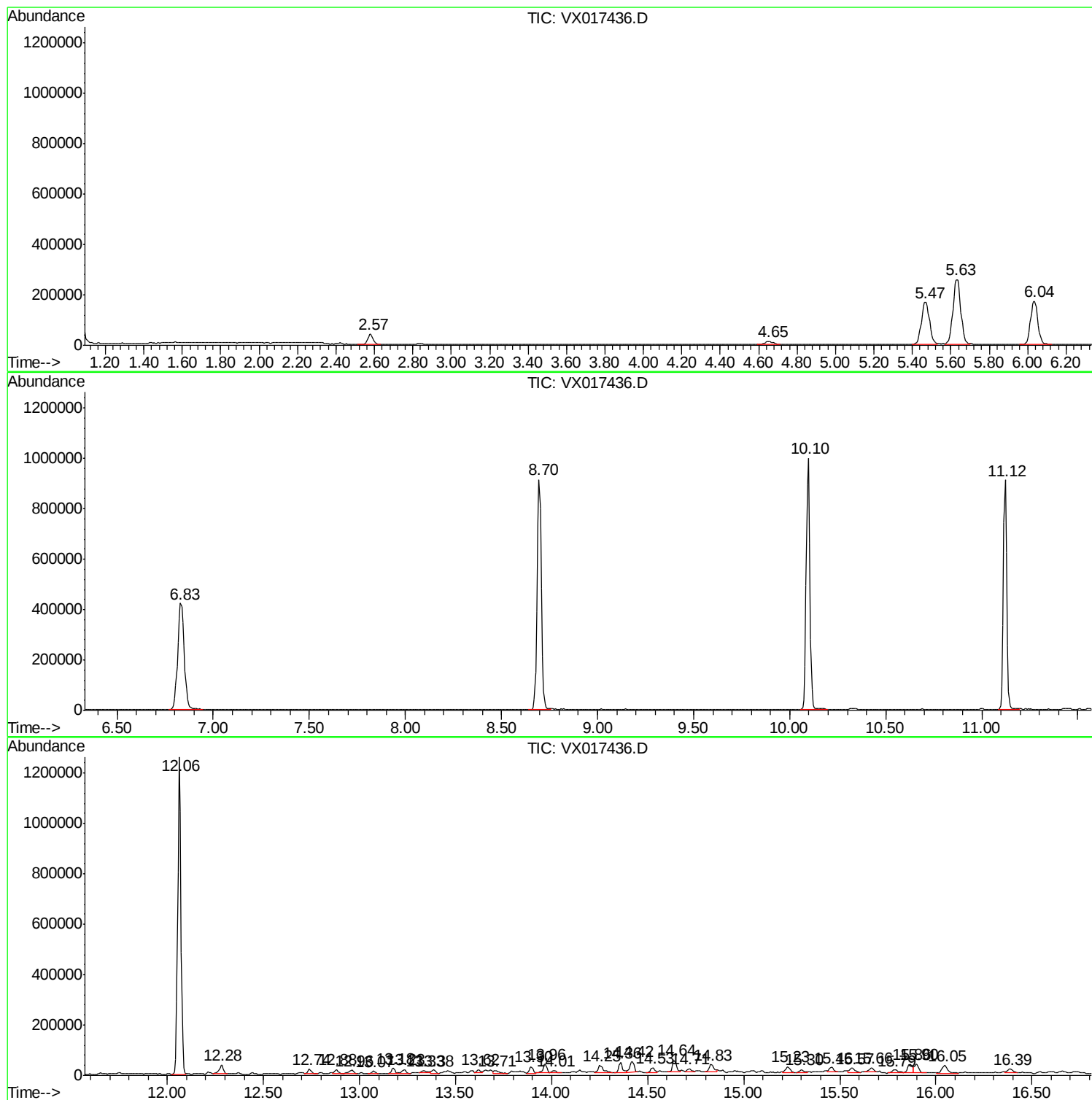
Sum of corrected areas: 9298047

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X071320W.M  
Quant Title : SW846 8260

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



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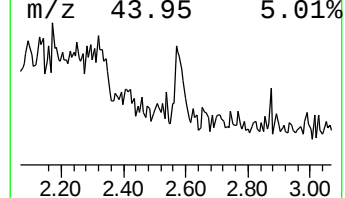
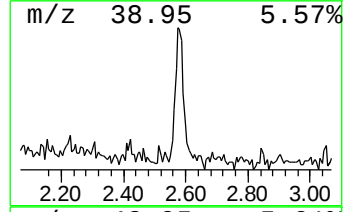
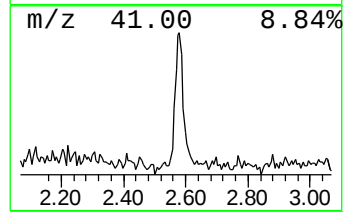
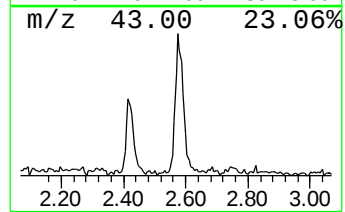
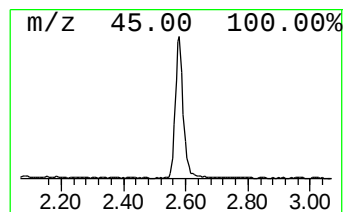
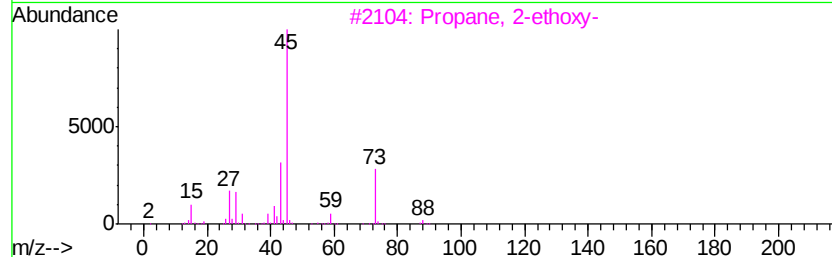
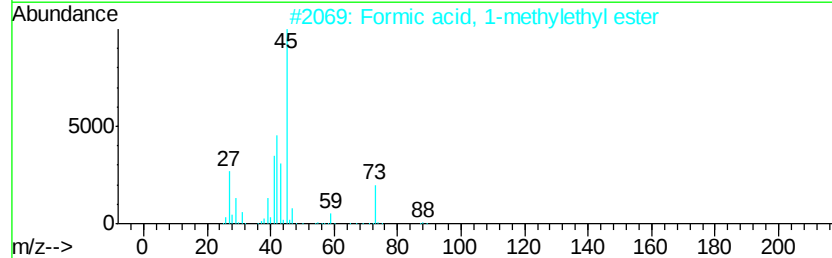
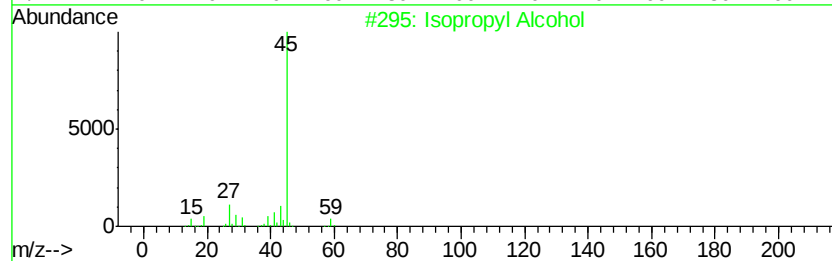
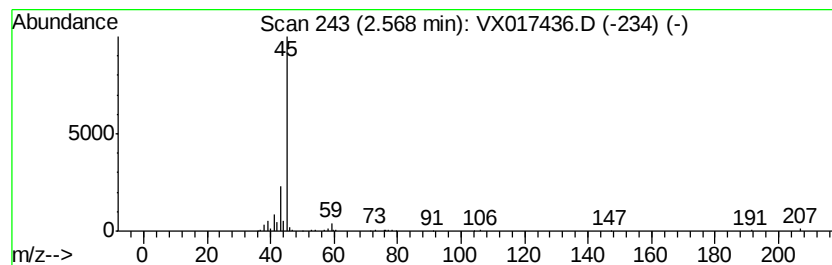
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X071320W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Isopropyl Alcohol Concentration Rank 1

| R.T. | EstConc   | Area  | Relative to ISTD   | R.T. |
|------|-----------|-------|--------------------|------|
| 2.57 | 5.72 ug/l | 81928 | Pentafluorobenzene | 5.63 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | Isopropyl Alcohol                | 60  | C3H8O   | 000067-63-0 | 72   |
| 2    |    | Formic acid, 1-methylethyl ester | 88  | C4H8O2  | 000625-55-8 | 40   |
| 3    |    | Propane, 2-ethoxy-               | 88  | C5H12O  | 000625-54-7 | 40   |
| 4    |    | (2R,4R)-(-)-Pentanediol          | 104 | C5H12O2 | 042075-32-1 | 9    |
| 5    |    | (R)-(-)-2-Pentanol               | 88  | C5H12O  | 031087-44-2 | 9    |



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| TIC Top Hit name  | RT   | EstConc | Units | Response | ---Internal Standard--- |      |        |      |
|-------------------|------|---------|-------|----------|-------------------------|------|--------|------|
|                   |      |         |       |          | #                       | RT   | Resp   | Conc |
| Isopropyl Alcohol | 2.57 | 5.7     | ug/l  | 81928    | 1                       | 5.63 | 716362 | 50.0 |