

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX020822\  
 Data File : VX026834.D  
 Acq On : 08 Feb 2022 19:52  
 Operator : JC/MD  
 Sample : N1400-02  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 25 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 KTS1-WC-L-MH-02

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\82X020822W.M  
 Title : SW846 8260

Signal : TIC: VX026834.D\data.ms

| 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         | 1.148       | 6             | 10          | 16           | rVB2     | 16618          | 17278         | 2.47%           | 0.446%        |
| 2         | 1.453       | 52            | 60          | 63           | rBV2     | 6412           | 11873         | 1.70%           | 0.307%        |
| 3         | 2.386       | 208           | 213         | 220          | rVB      | 5089           | 8594          | 1.23%           | 0.222%        |
| 4         | 2.544       | 229           | 239         | 250          | rBV2     | 3692           | 11939         | 1.70%           | 0.308%        |
| 5         | 5.391       | 694           | 706         | 722          | rBV      | 83794          | 242849        | 34.67%          | 6.270%        |
| 6         | 5.562       | 722           | 734         | 748          | rVV      | 146473         | 412653        | 58.92%          | 10.654%       |
| 7         | 5.964       | 789           | 800         | 811          | rBV      | 93307          | 245530        | 35.06%          | 6.339%        |
| 8         | 6.763       | 919           | 931         | 947          | rBV      | 227679         | 540042        | 77.11%          | 13.943%       |
| 9         | 8.653       | 1234          | 1241        | 1250         | rBV      | 449647         | 700364        | 100.00%         | 18.082%       |
| 10        | 10.055      | 1465          | 1471        | 1479         | rBV      | 446946         | 593749        | 84.78%          | 15.329%       |
| 11        | 11.079      | 1634          | 1639        | 1645         | rBV      | 334285         | 438507        | 62.61%          | 11.321%       |
| 12        | 12.024      | 1788          | 1794        | 1803         | rVB      | 435434         | 529741        | 75.64%          | 13.677%       |
| 13        | 13.146      | 1972          | 1978        | 1983         | rBV      | 56669          | 72655         | 10.37%          | 1.876%        |
| 14        | 14.371      | 2174          | 2179        | 2185         | rBV6     | 4076           | 7599          | 1.09%           | 0.196%        |
| 15        | 14.792      | 2244          | 2248        | 2251         | rVB2     | 7524           | 9041          | 1.29%           | 0.233%        |
| 16        | 15.188      | 2306          | 2313        | 2320         | rVB7     | 6029           | 14614         | 2.09%           | 0.377%        |
| 17        | 15.664      | 2386          | 2391        | 2397         | rBV6     | 3655           | 7555          | 1.08%           | 0.195%        |
| 18        | 15.737      | 2398          | 2403        | 2408         | rVB3     | 4793           | 8727          | 1.25%           | 0.225%        |

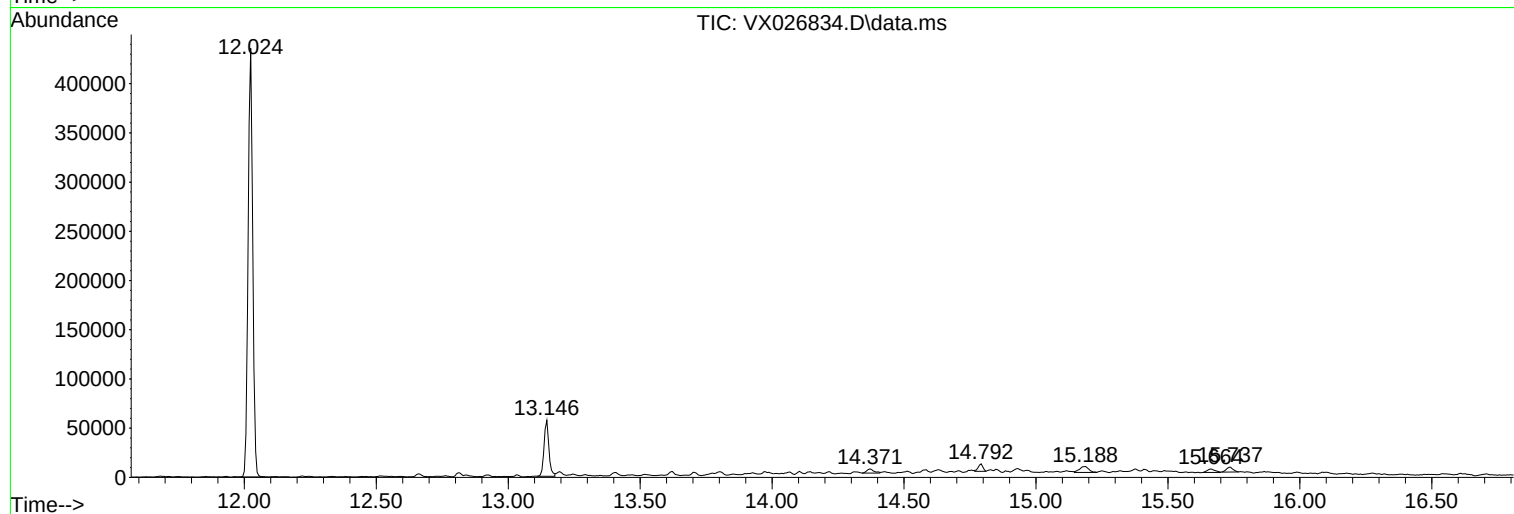
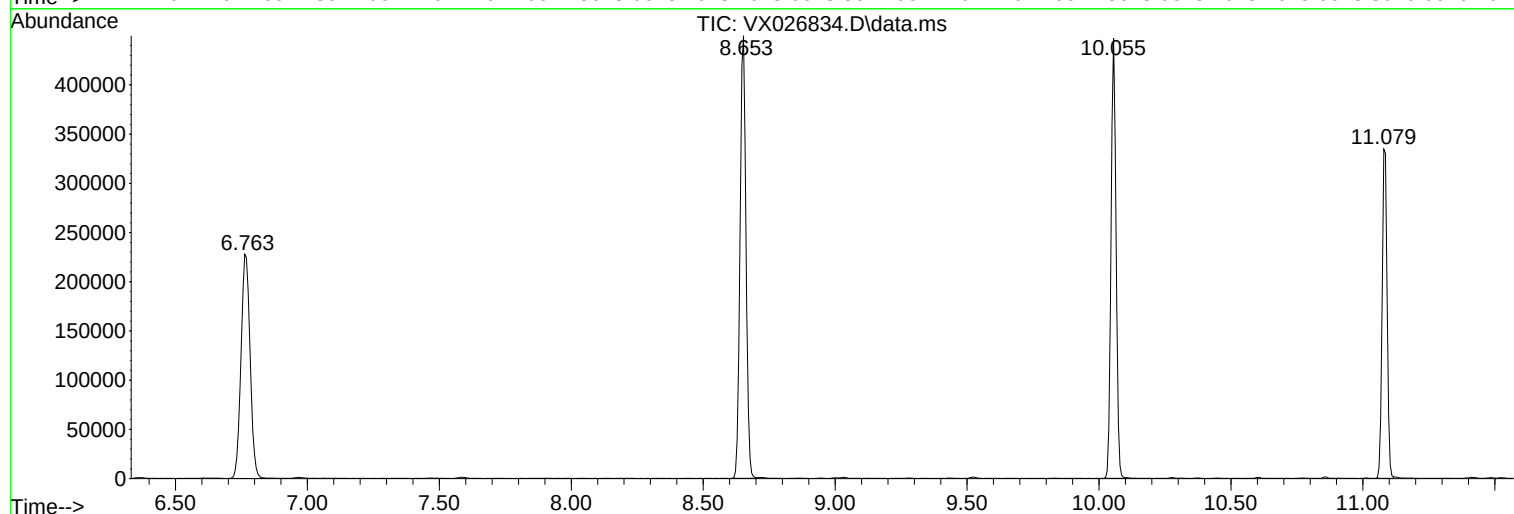
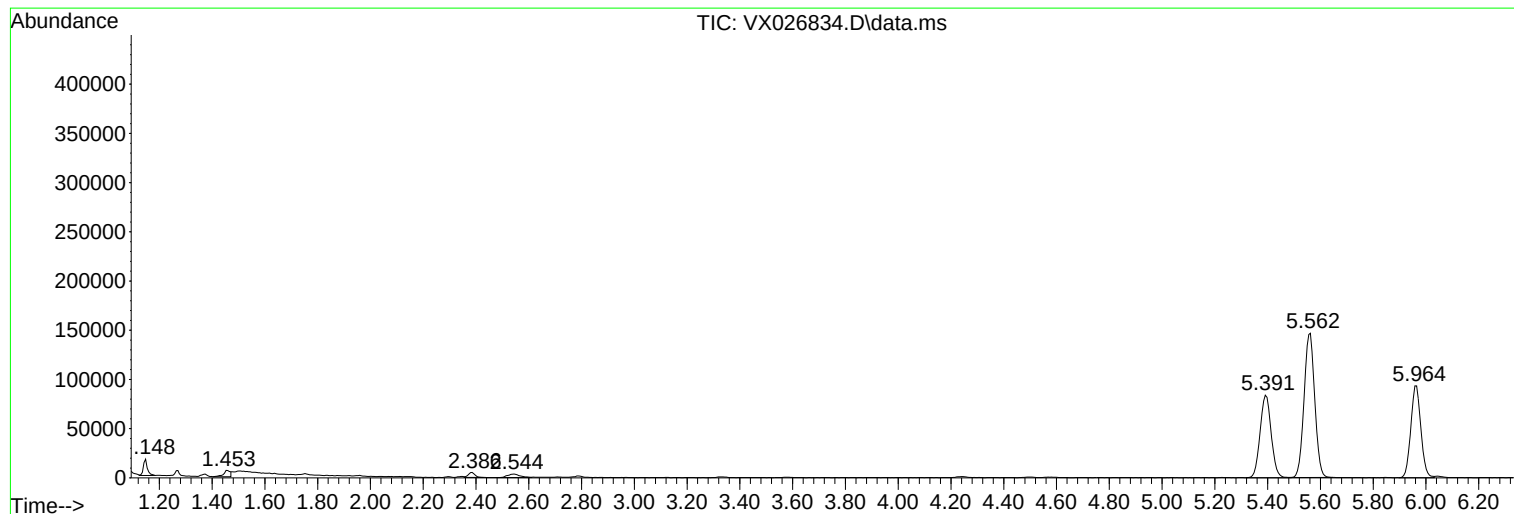
Sum of corrected areas: 3873310

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KTS1-WC-L-MH-02

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X020822W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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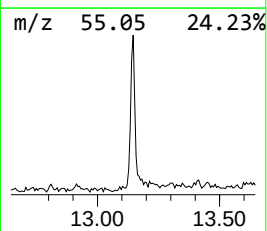
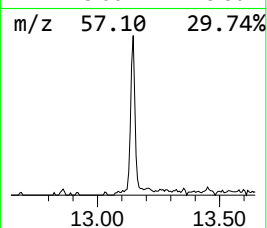
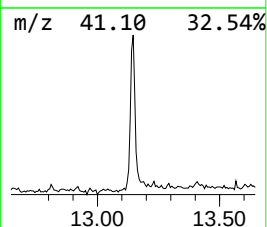
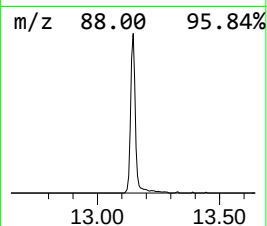
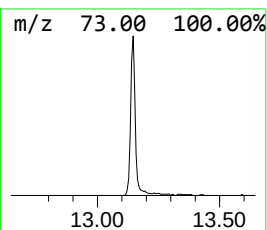
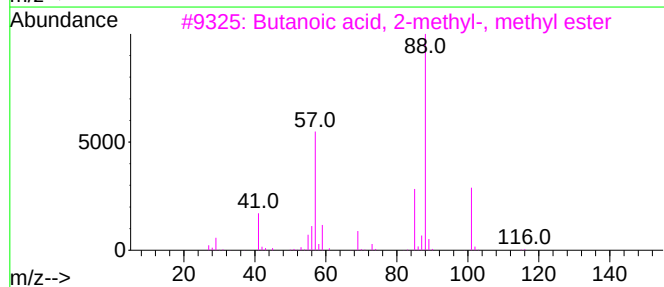
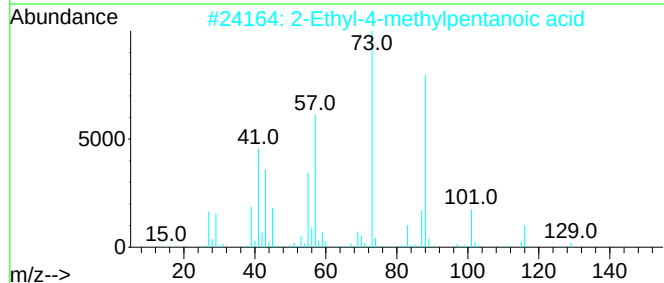
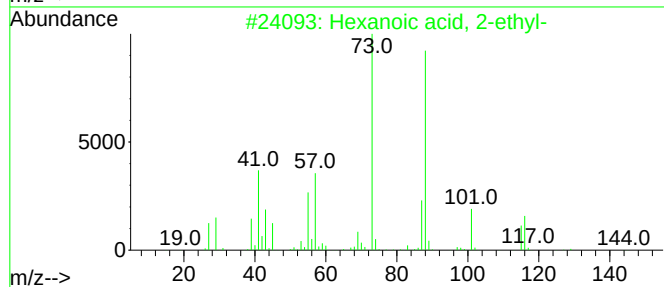
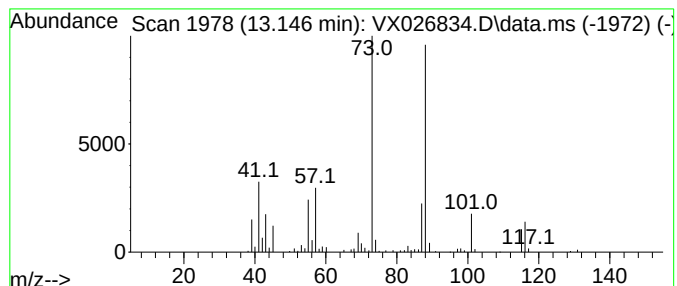
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X020822W.M  
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TIC Integration Parameters: LSCINT.P

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Peak Number 1 Hexanoic acid, 2-ethyl- Concentration Rank 1

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 13.146 | 6.86 ug/l | 72655 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Hexanoic acid, 2-ethyl-             | 144 | C8H16O2  | 000149-57-5 | 91   |
| 2    |    |   | 2-Ethyl-4-methylpentanoic acid      | 144 | C8H16O2  | 000108-81-6 | 56   |
| 3    |    |   | Butanoic acid, 2-methyl-, methyl... | 116 | C6H12O2  | 000868-57-5 | 47   |
| 4    |    |   | Methyl 2,3,4-tri-O-methyl-6-deox... | 220 | C10H20O5 | 072983-16-5 | 42   |
| 5    |    |   | Heptanoic acid, 2-ethyl-            | 158 | C9H18O2  | 003274-29-1 | 42   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Hexanoic acid, ... | 13.146 | 6.9     | ug/l  | 72655    | 4                     | 12.024 | 529741 | 50.0 |