

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX091522\  
 Data File : VX031367.D  
 Acq On : 15 Sep 2022 20:29  
 Operator : JC/MD  
 Sample : N4508-05  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 BR-01-180-200-090122

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\82X091422W.M  
 Title : SW846 8260

Signal : TIC: VX031367.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         | 1.569       | 72            | 79          | 80           | rBV6     | 7306           | 11583         | 1.38%           | 0.296%        |
| 2         | 2.319       | 197           | 202         | 209          | rVB      | 44356          | 68469         | 8.18%           | 1.753%        |
| 3         | 2.514       | 227           | 234         | 247          | rBV      | 70827          | 115901        | 13.85%          | 2.967%        |
| 4         | 2.947       | 297           | 305         | 317          | rBV      | 10903          | 26316         | 3.14%           | 0.674%        |
| 5         | 4.495       | 549           | 559         | 565          | rBV2     | 6993           | 18406         | 2.20%           | 0.471%        |
| 6         | 4.574       | 565           | 572         | 587          | rVB      | 5890           | 19006         | 2.27%           | 0.487%        |
| 7         | 5.092       | 647           | 657         | 669          | rBV3     | 14292          | 43297         | 5.17%           | 1.108%        |
| 8         | 5.391       | 693           | 706         | 721          | rBV      | 99127          | 286696        | 34.25%          | 7.339%        |
| 9         | 5.556       | 721           | 733         | 746          | rVB      | 97361          | 271856        | 32.48%          | 6.959%        |
| 10        | 5.958       | 789           | 799         | 812          | rBV      | 109813         | 291288        | 34.80%          | 7.456%        |
| 11        | 6.763       | 921           | 931         | 944          | rBV      | 153509         | 364528        | 43.55%          | 9.331%        |
| 12        | 7.129       | 983           | 991         | 1001         | rVB2     | 18731          | 42006         | 5.02%           | 1.075%        |
| 13        | 8.653       | 1234          | 1241        | 1248         | rBV      | 535991         | 836956        | 100.00%         | 21.424%       |
| 14        | 8.720       | 1248          | 1252        | 1263         | rVB      | 18074          | 29317         | 3.50%           | 0.750%        |
| 15        | 10.055      | 1465          | 1471        | 1478         | rBV      | 339023         | 439676        | 52.53%          | 11.254%       |
| 16        | 11.079      | 1634          | 1639        | 1646         | rBV      | 421784         | 541411        | 64.69%          | 13.859%       |
| 17        | 12.024      | 1789          | 1794        | 1801         | rBV      | 334043         | 406357        | 48.55%          | 10.402%       |
| 18        | 12.219      | 1820          | 1826        | 1845         | rBV      | 44240          | 93601         | 11.18%          | 2.396%        |

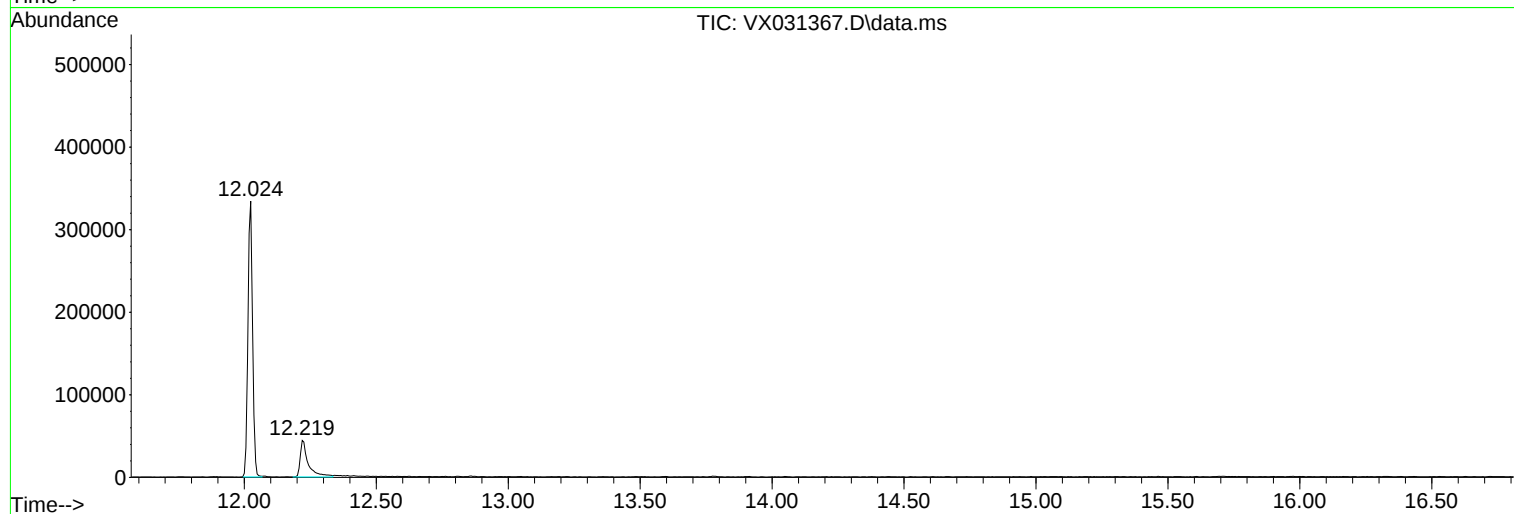
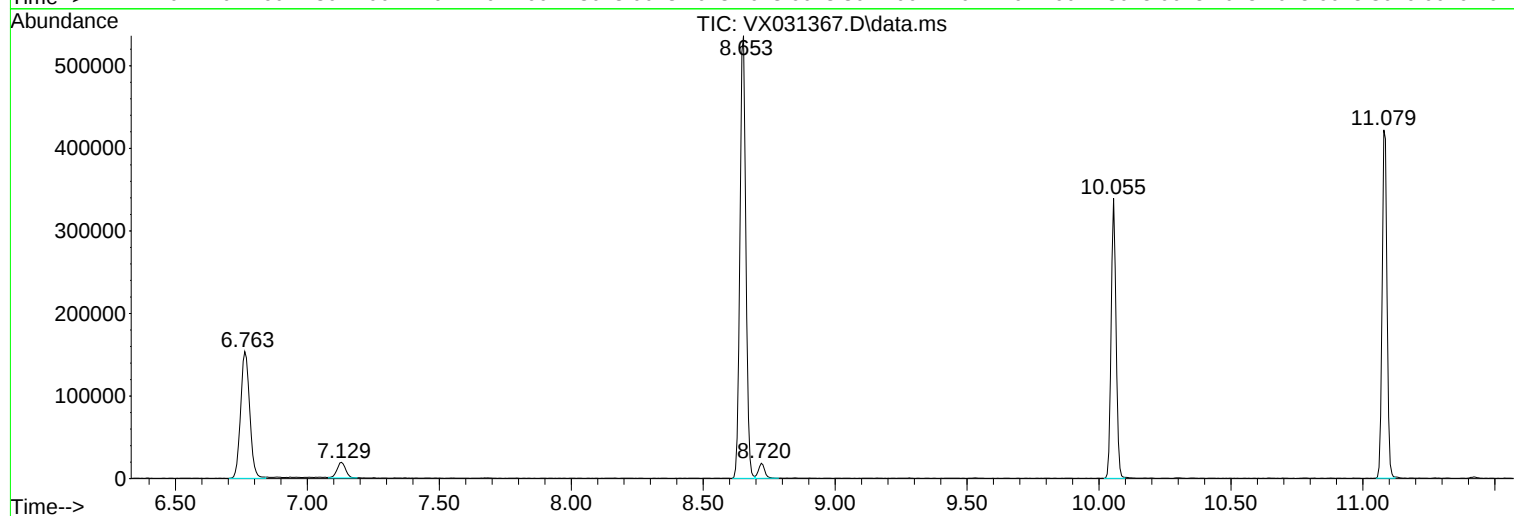
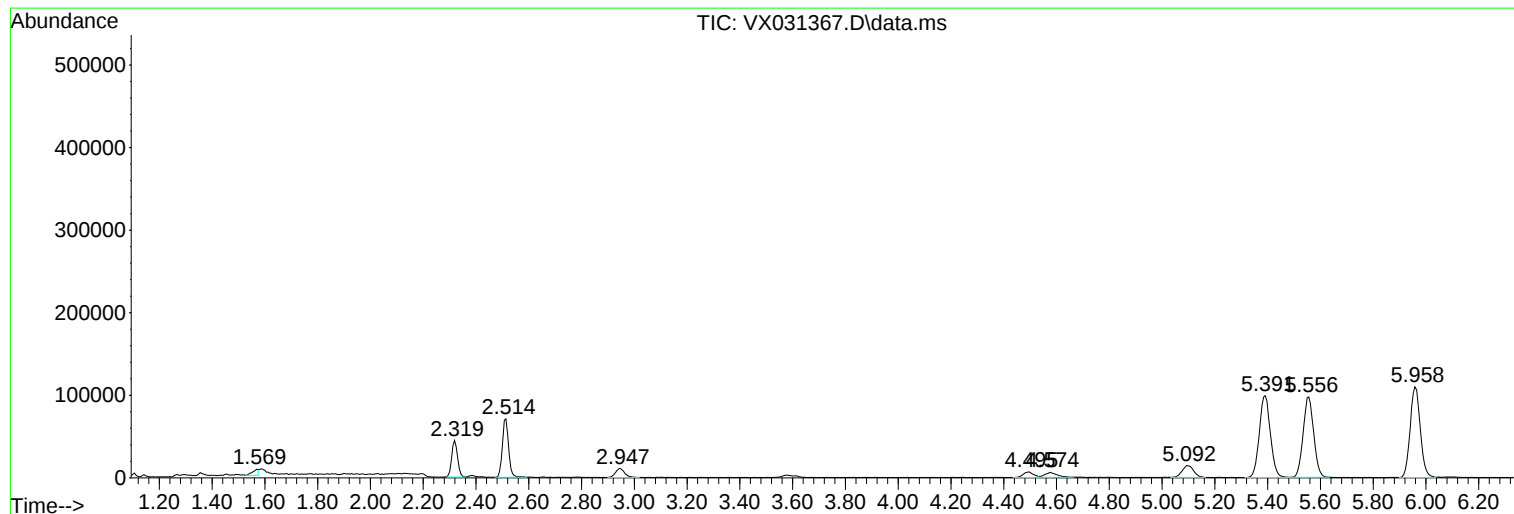
Sum of corrected areas: 3906670

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BR-01-180-200-090122

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091422W.M  
Quant Title : SW846 8260

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



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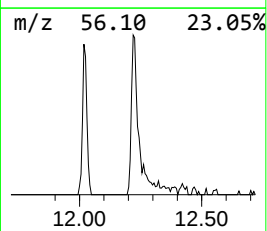
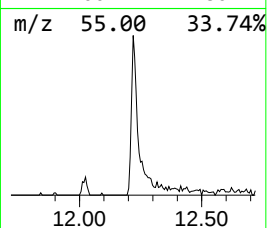
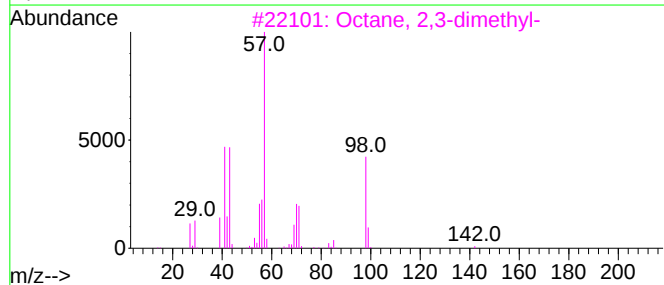
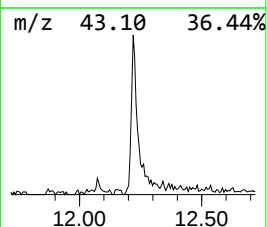
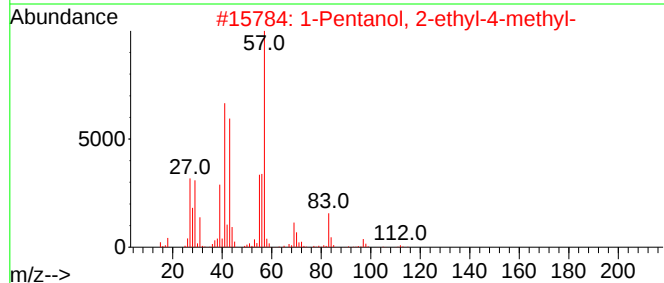
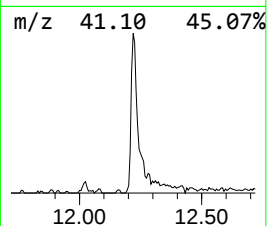
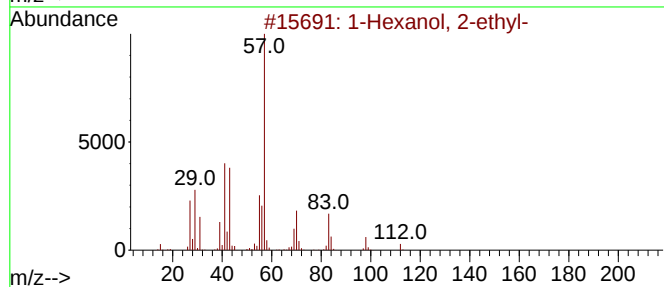
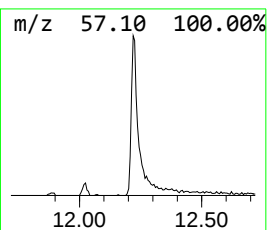
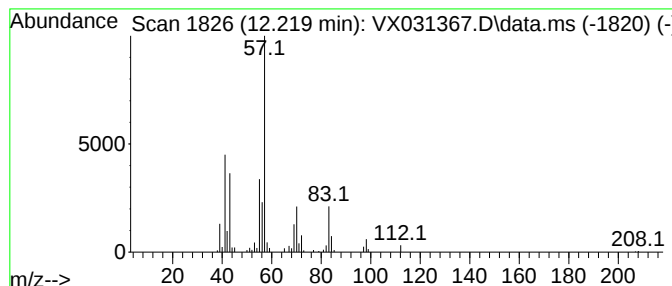
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091422W.M  
Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

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

| R.T.   | EstConc    | Area  | Relative to ISTD       | R.T.   |
|--------|------------|-------|------------------------|--------|
| 12.219 | 11.52 ug/l | 93601 | 1,4-Dichlorobenzene-d4 | 12.024 |

| Hit# | of                                | 5 | Tentative ID | MW  | MolForm  | CAS#         | Qual |
|------|-----------------------------------|---|--------------|-----|----------|--------------|------|
| 1    | 1-Hexanol, 2-ethyl-               |   |              | 130 | C8H18O   | 000104-76-7  | 80   |
| 2    | 1-Pentanol, 2-ethyl-4-methyl-     |   |              | 130 | C8H18O   | 000106-67-2  | 59   |
| 3    | Octane, 2,3-dimethyl-             |   |              | 142 | C10H22   | 007146-60-3  | 53   |
| 4    | Heptyl isobutyl carbonate         |   |              | 216 | C12H24O3 | 959068-08-7  | 53   |
| 5    | Carbonic acid, butyl heptyl ester |   |              | 216 | C12H24O3 | 1000314-63-4 | 50   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 1-Hexanol, 2-et... | 12.219 | 11.5    | ug/l  | 93601    | 4                     | 12.024 | 406357 | 50.0 |