

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX040425\  
 Data File : VX045593.D  
 Acq On : 04 Apr 2025 12:50  
 Operator : JC/MD  
 Sample : Q1716-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 MOD-FOR-LRSA

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\82X040225W.M  
 Title : SW846 8260

Signal : TIC: VX045593.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         | 1.538       | 70            | 74          | 78           | rBV      | 55461          | 54661         | 11.98%          | 2.144%        |
| 2         | 1.611       | 83            | 86          | 89           | rVB3     | 5241           | 7327          | 1.61%           | 0.287%        |
| 3         | 2.550       | 230           | 240         | 253          | rBV      | 12801          | 25228         | 5.53%           | 0.989%        |
| 4         | 2.782       | 273           | 278         | 285          | rBV3     | 2946           | 5440          | 1.19%           | 0.213%        |
| 5         | 2.940       | 297           | 304         | 313          | rBV2     | 4117           | 9383          | 2.06%           | 0.368%        |
| 6         | 5.385       | 694           | 705         | 720          | rBV      | 53599          | 159493        | 34.96%          | 6.256%        |
| 7         | 5.544       | 720           | 731         | 745          | rVV      | 75990          | 216565        | 47.47%          | 8.494%        |
| 8         | 5.952       | 788           | 798         | 812          | rBV      | 63409          | 168468        | 36.93%          | 6.608%        |
| 9         | 6.757       | 922           | 930         | 953          | rBV      | 134489         | 326935        | 71.66%          | 12.823%       |
| 10        | 8.647       | 1233          | 1240        | 1253         | rBV      | 285909         | 456218        | 100.00%         | 17.894%       |
| 11        | 9.531       | 1381          | 1385        | 1395         | rBV3     | 3394           | 6198          | 1.36%           | 0.243%        |
| 12        | 10.049      | 1465          | 1470        | 1486         | rBV      | 285160         | 410781        | 90.04%          | 16.112%       |
| 13        | 11.079      | 1634          | 1639        | 1655         | rBV      | 232652         | 301482        | 66.08%          | 11.825%       |
| 14        | 12.018      | 1788          | 1793        | 1805         | rBV      | 272891         | 354177        | 77.63%          | 13.892%       |
| 15        | 12.219      | 1819          | 1826        | 1836         | rBV      | 27692          | 47237         | 10.35%          | 1.853%        |

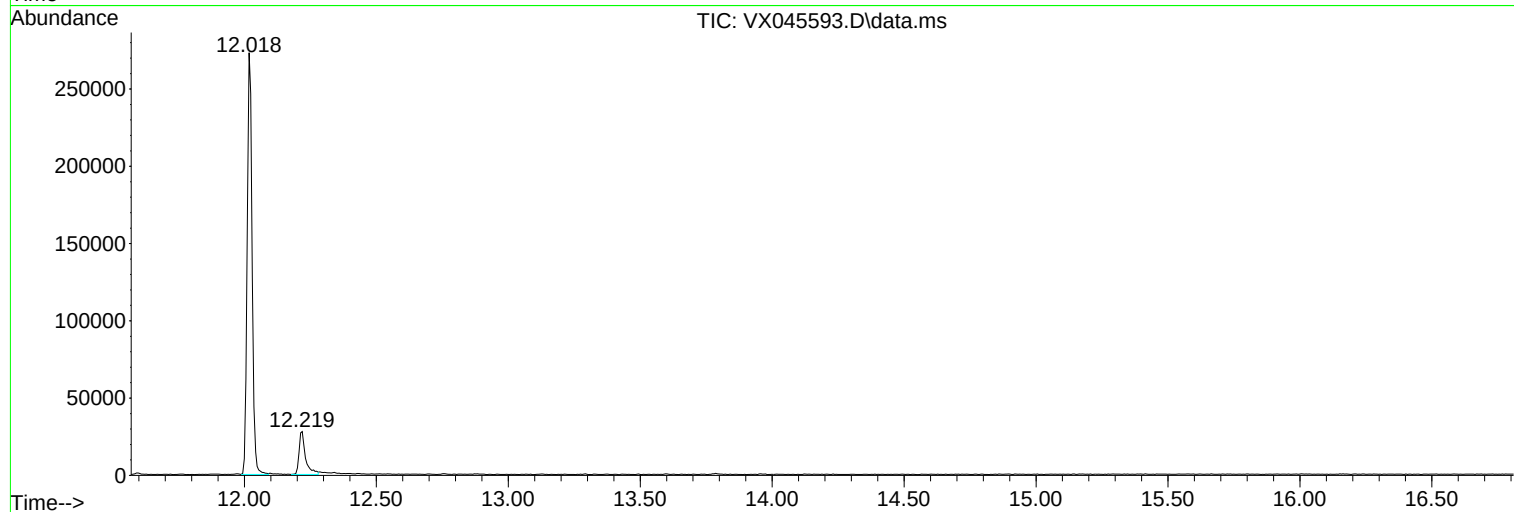
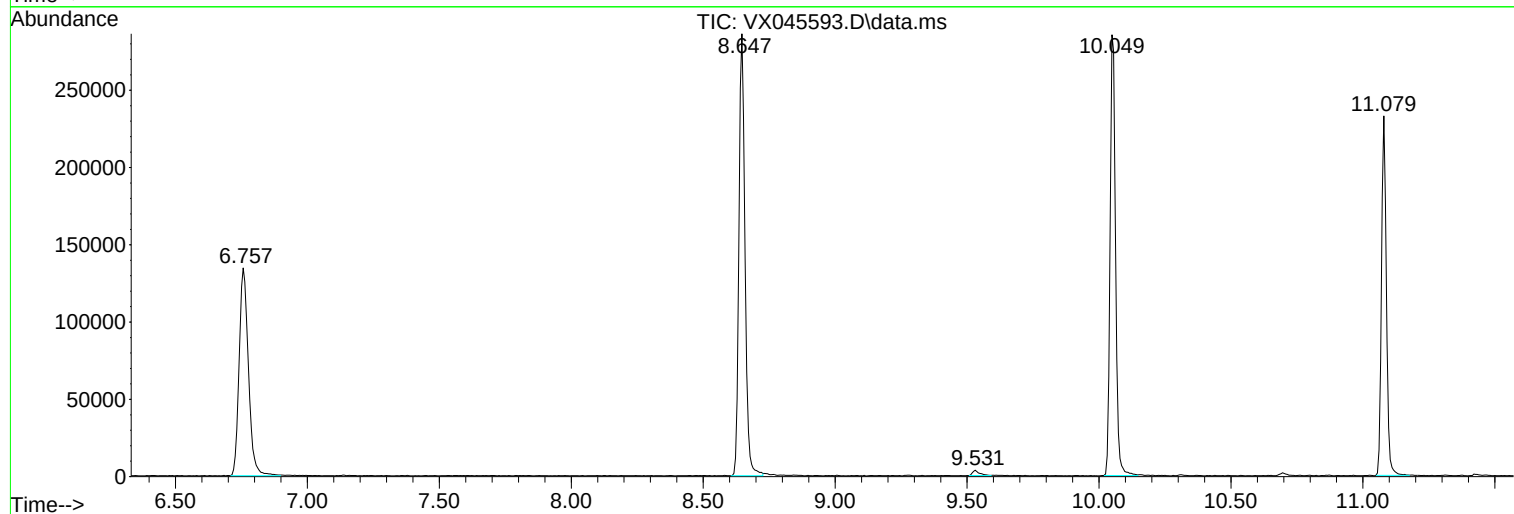
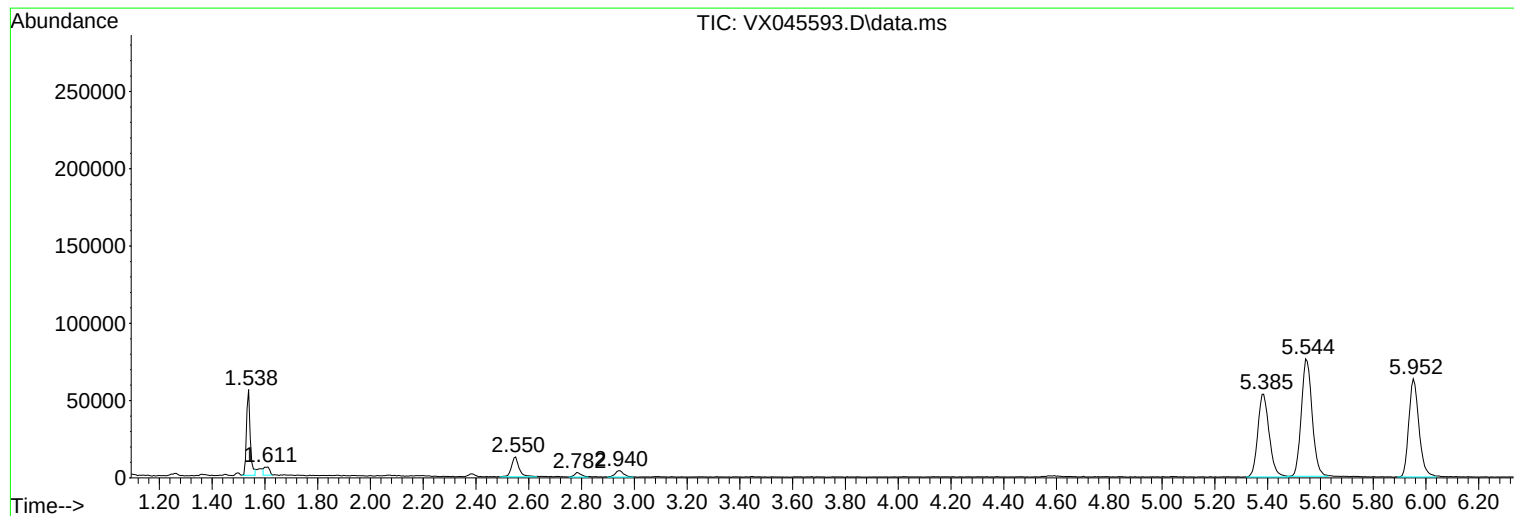
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X040225W.M  
Quant Title : SW846 8260

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



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ClientSampleId :  
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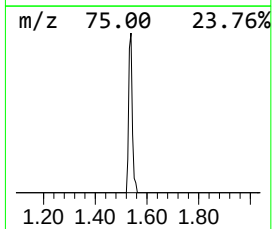
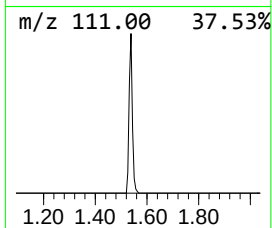
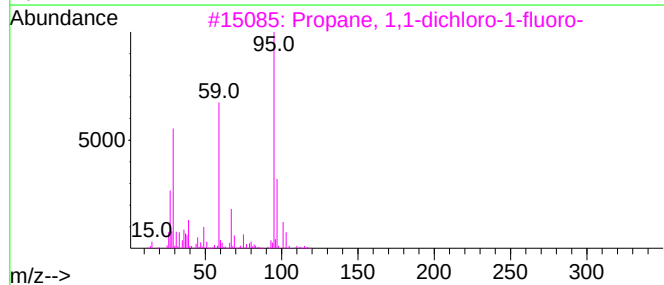
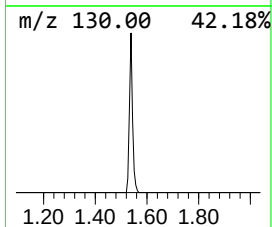
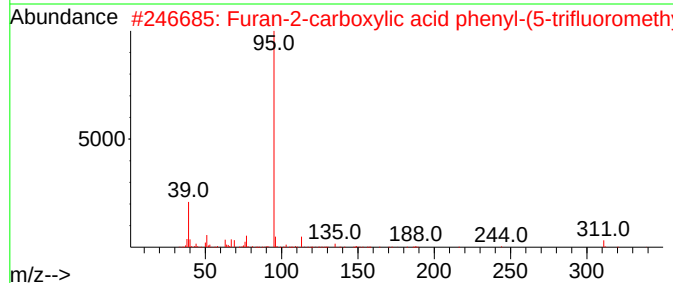
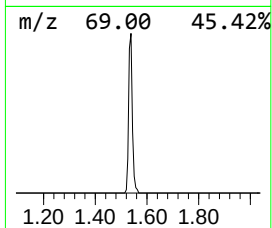
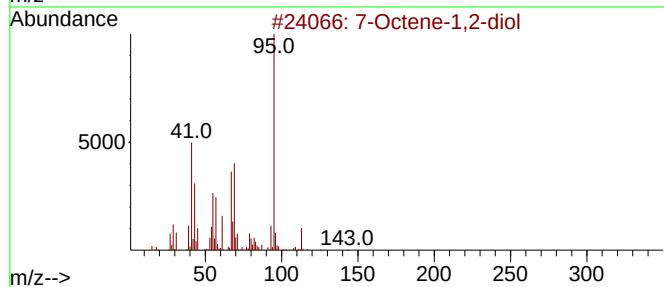
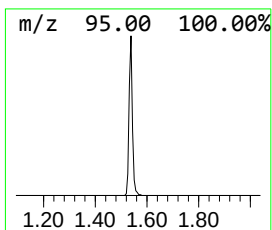
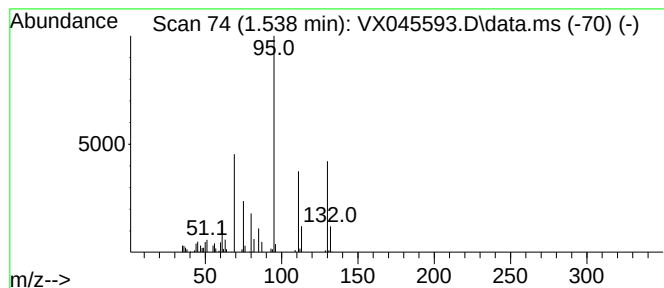
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X040225W.M  
Quant Title : SW846 8260

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

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Peak Number 1 unknown1.538 Concentration Rank 1

| R.T.  | EstConc    | Area  | Relative to ISTD   | R.T.  |
|-------|------------|-------|--------------------|-------|
| 1.538 | 12.62 ug/l | 54661 | Pentafluorobenzene | 5.550 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm      | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|--------------|--------------|------|
| 1    |    |   | 7-Octene-1,2-diol                   | 144 | C8H16O2      | 085866-02-0  | 23   |
| 2    |    |   | Furan-2-carboxylic acid phenyl-(... | 339 | C14H8F3N3O2S | 1000300-94-9 | 12   |
| 3    |    |   | Propane, 1,1-dichloro-1-fluoro-     | 130 | C3H5Cl2F     | 007799-56-6  | 10   |
| 4    |    |   | Pyridine, 1-oxide                   | 95  | C5H5NO       | 000694-59-7  | 9    |
| 5    |    |   | 3-Pyridinol                         | 95  | C5H5NO       | 000109-00-2  | 9    |



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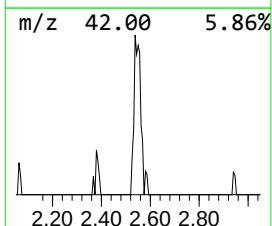
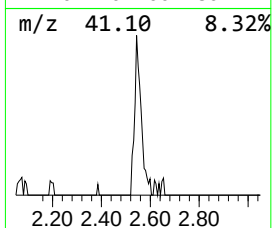
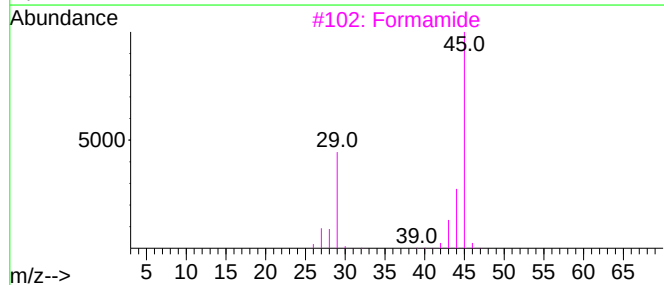
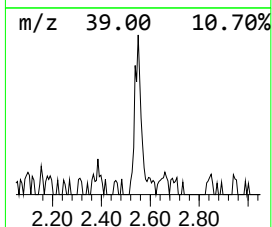
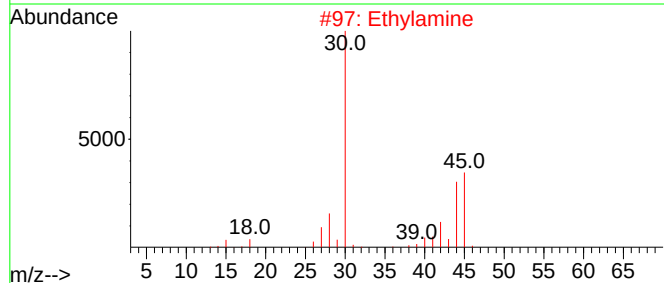
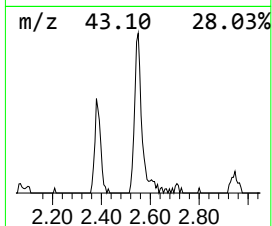
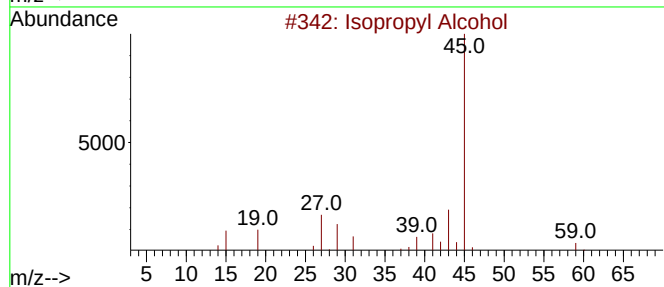
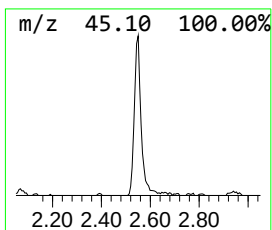
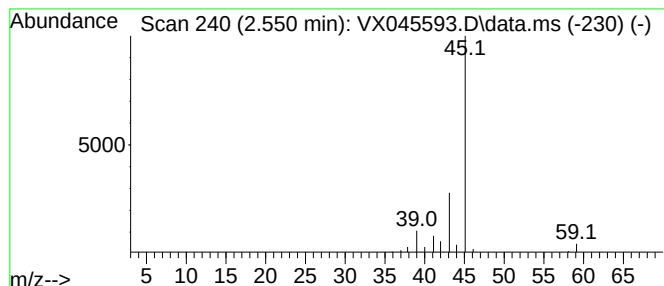
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Peak Number 2 Isopropyl Alcohol Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 2.550 | 5.82 ug/l | 25228 | Pentafluorobenzene | 5.550 |

| Hit# | of 5 | Tentative ID              | MW | MolForm | CAS#        | Qual |
|------|------|---------------------------|----|---------|-------------|------|
| 1    |      | Isopropyl Alcohol         | 60 | C3H8O   | 000067-63-0 | 74   |
| 2    |      | Ethylamine                | 45 | C2H7N   | 000075-04-7 | 4    |
| 3    |      | Formamide                 | 45 | CH3NO   | 000075-12-7 | 4    |
| 4    |      | Oxirane, (methoxymethyl)- | 88 | C4H8O2  | 000930-37-0 | 4    |
| 5    |      | 2-Propanone, 1-methoxy-   | 88 | C4H8O2  | 005878-19-3 | 4    |



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MSVOA\_X  
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MOD-FOR-LRSA

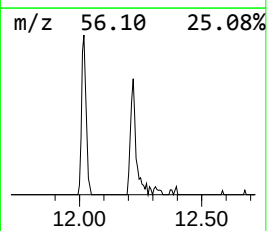
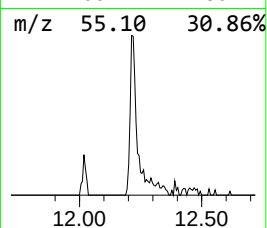
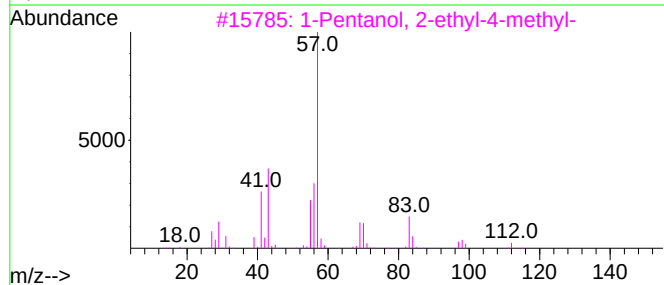
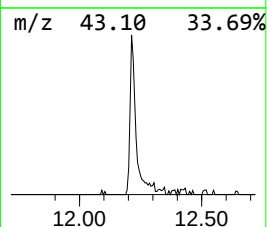
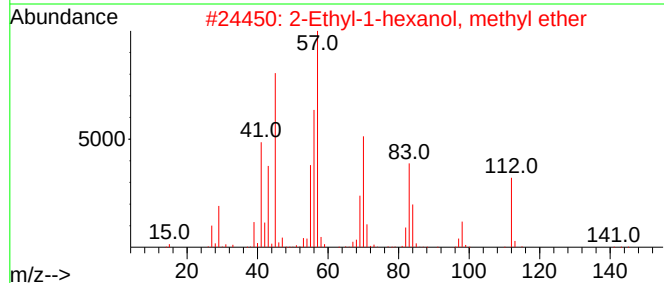
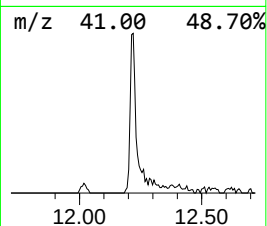
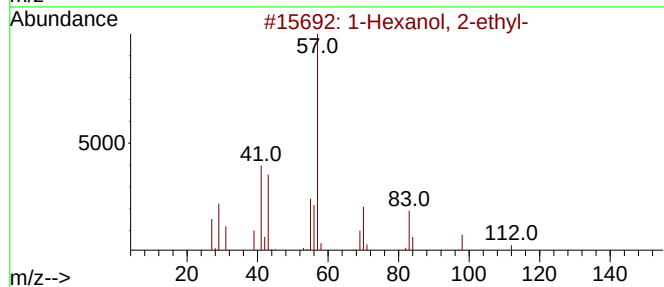
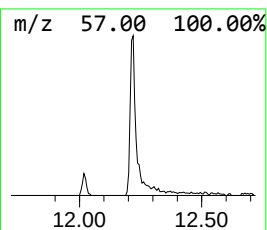
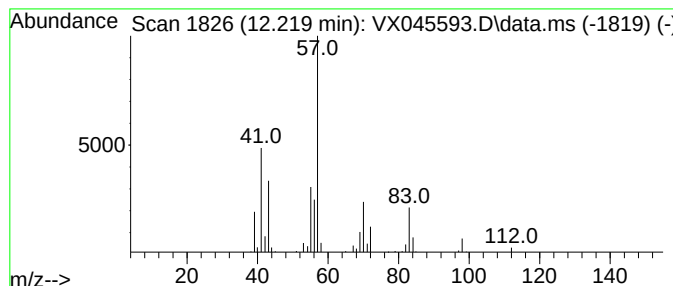
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X040225W.M  
Quant Title : SW846 8260

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

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Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 12.219 | 6.67 ug/l | 47237 | 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  | 86   |
| 2    |    |   | 2-Ethyl-1-hexanol, methyl ether | 144 | C9H20O   | 1000365-10-2 | 53   |
| 3    |    |   | 1-Pentanol, 2-ethyl-4-methyl-   | 130 | C8H18O   | 000106-67-2  | 53   |
| 4    |    |   | 2-Propyl-1-pentanol             | 130 | C8H18O   | 058175-57-8  | 50   |
| 5    |    |   | Heptyl isobutyl carbonate       | 216 | C12H24O3 | 959068-08-7  | 43   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| unknown1.538       | 1.538  | 12.6    | ug/l  | 54661    | 1                     | 5.550  | 216565 | 50.0 |
| Isopropyl Alcohol  | 2.550  | 5.8     | ug/l  | 25228    | 1                     | 5.550  | 216565 | 50.0 |
| 1-Hexanol, 2-et... | 12.219 | 6.7     | ug/l  | 47237    | 4                     | 12.024 | 354177 | 50.0 |