

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN050222\  
 Data File : VN072299.D  
 Acq On : 02 May 2022 17:11  
 Operator : JC\MD  
 Sample : N2653-08  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 30992

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\82N042622W.M  
 Title : SW846 8260

Signal : TIC: VN072299.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         | 2.034       | 3             | 8           | 13           | rBV      | 23516          | 34107         | 2.16%           | 0.297%        |
| 2         | 2.240       | 36            | 43          | 46           | rBV2     | 27706          | 62795         | 3.98%           | 0.547%        |
| 3         | 2.587       | 95            | 102         | 112          | rBV      | 50042          | 86074         | 5.46%           | 0.750%        |
| 4         | 3.681       | 272           | 288         | 308          | rBV      | 570822         | 1576515       | 100.00%         | 13.739%       |
| 5         | 4.287       | 383           | 391         | 399          | rBV2     | 18462          | 52414         | 3.32%           | 0.457%        |
| 6         | 5.963       | 668           | 676         | 687          | rVB5     | 8722           | 27044         | 1.72%           | 0.236%        |
| 7         | 7.057       | 849           | 862         | 878          | rBV      | 505547         | 1467418       | 93.08%          | 12.788%       |
| 8         | 7.328       | 899           | 908         | 917          | rBV      | 70431          | 179713        | 11.40%          | 1.566%        |
| 9         | 8.016       | 1015          | 1025        | 1030         | rBV2     | 146717         | 341968        | 21.69%          | 2.980%        |
| 10        | 8.081       | 1030          | 1036        | 1050         | rVB      | 297326         | 688981        | 43.70%          | 6.004%        |
| 11        | 8.434       | 1084          | 1096        | 1109         | rBV2     | 187338         | 503703        | 31.95%          | 4.390%        |
| 12        | 8.963       | 1177          | 1186        | 1202         | rBV      | 403634         | 840901        | 53.34%          | 7.328%        |
| 13        | 9.151       | 1210          | 1218        | 1233         | rBV      | 54415          | 144707        | 9.18%           | 1.261%        |
| 14        | 9.528       | 1275          | 1282        | 1295         | rBV2     | 71756          | 145907        | 9.26%           | 1.272%        |
| 15        | 10.439      | 1427          | 1437        | 1443         | rBV      | 611693         | 1109464       | 70.37%          | 9.668%        |
| 16        | 10.498      | 1443          | 1447        | 1457         | rVV      | 148683         | 281285        | 17.84%          | 2.451%        |
| 17        | 10.598      | 1458          | 1464        | 1470         | rVB6     | 7430           | 15805         | 1.00%           | 0.138%        |
| 18        | 10.857      | 1499          | 1508        | 1519         | rBV2     | 44886          | 115218        | 7.31%           | 1.004%        |
| 19        | 11.739      | 1646          | 1658        | 1670         | rBV      | 561552         | 1046300       | 66.37%          | 9.118%        |
| 20        | 11.839      | 1670          | 1675        | 1681         | rVB2     | 12903          | 20129         | 1.28%           | 0.175%        |
| 21        | 11.945      | 1687          | 1693        | 1702         | rBV      | 28769          | 53189         | 3.37%           | 0.464%        |
| 22        | 12.275      | 1743          | 1749        | 1752         | rBV4     | 17701          | 32277         | 2.05%           | 0.281%        |
| 23        | 12.316      | 1752          | 1756        | 1764         | rVB      | 39256          | 68590         | 4.35%           | 0.598%        |
| 24        | 12.727      | 1818          | 1826        | 1838         | rBV      | 378266         | 675261        | 42.83%          | 5.885%        |
| 25        | 13.139      | 1889          | 1896        | 1898         | rBV2     | 27150          | 51025         | 3.24%           | 0.445%        |
| 26        | 13.163      | 1898          | 1900        | 1906         | rVV3     | 27683          | 37295         | 2.37%           | 0.325%        |
| 27        | 13.227      | 1906          | 1911        | 1920         | rVB2     | 35205          | 54461         | 3.45%           | 0.475%        |
| 28        | 13.422      | 1939          | 1944        | 1956         | rVB      | 103901         | 189135        | 12.00%          | 1.648%        |
| 29        | 13.522      | 1956          | 1961        | 1967         | rBV5     | 15219          | 25254         | 1.60%           | 0.220%        |
| 30        | 13.669      | 1978          | 1986        | 1996         | rBV      | 412500         | 706649        | 44.82%          | 6.158%        |
| 31        | 13.769      | 1996          | 2003        | 2014         | rBV      | 447377         | 841516        | 53.38%          | 7.333%        |

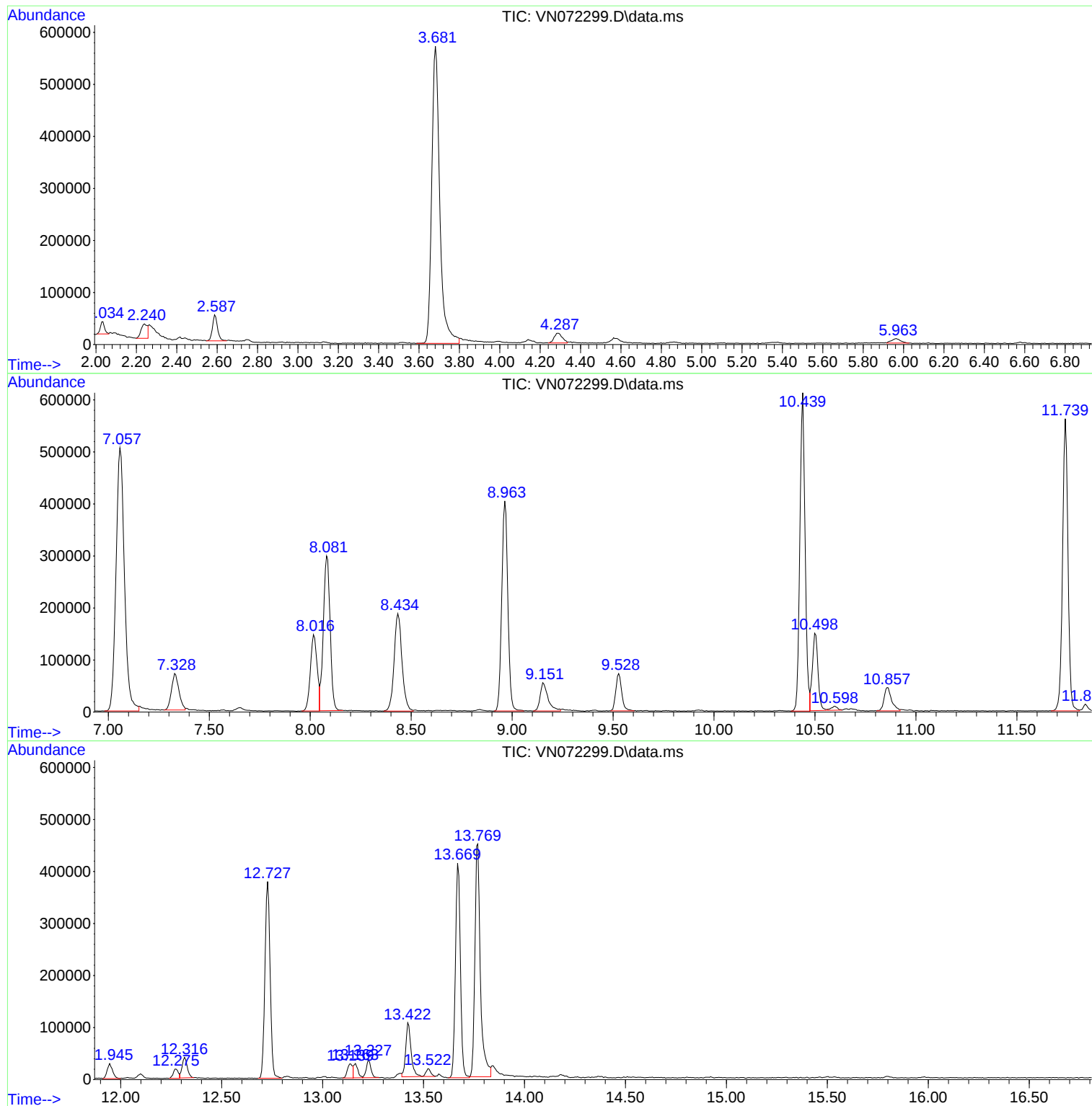
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

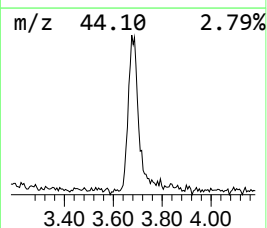
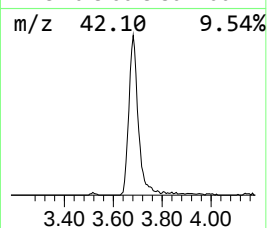
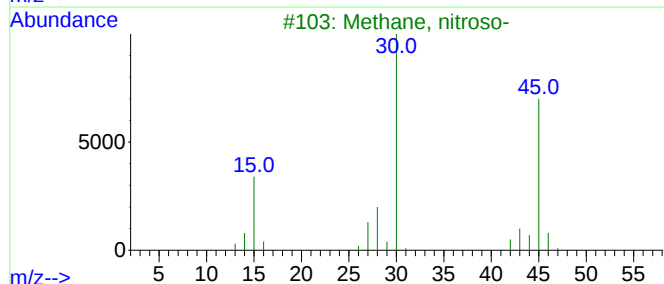
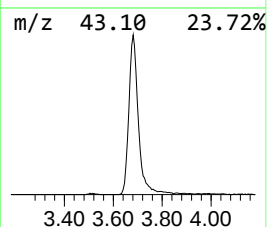
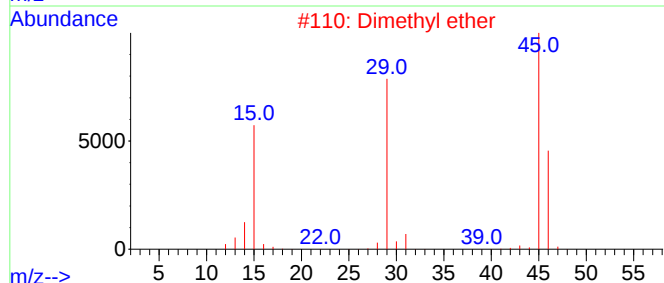
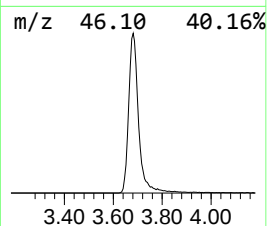
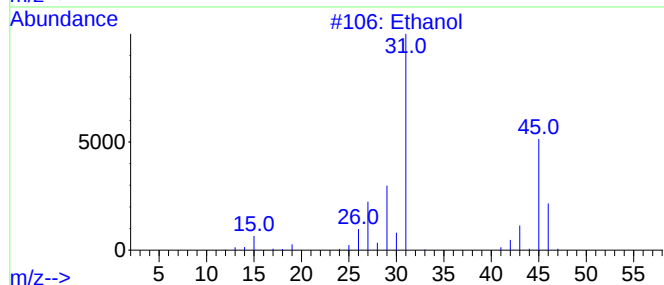
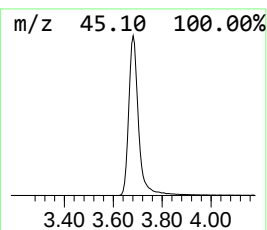
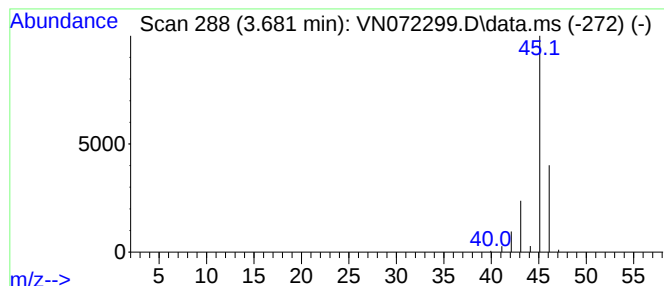
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Ethanol Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 3.681 | 114.41 ug/l | 1576520 | Pentafluorobenzene | 8.081 |

| Hit# | of | 5 | Tentative ID      | MW | MolForm | CAS#        | Qual |
|------|----|---|-------------------|----|---------|-------------|------|
| 1    |    |   | Ethanol           | 46 | C2H6O   | 000064-17-5 | 74   |
| 2    |    |   | Dimethyl ether    | 46 | C2H6O   | 000115-10-6 | 9    |
| 3    |    |   | Methane, nitroso- | 45 | CH3NO   | 000865-40-7 | 4    |
| 4    |    |   | Formic acid       | 46 | CH2O2   | 000064-18-6 | 4    |
| 5    |    |   | Oxalic acid       | 90 | C2H2O4  | 000144-62-7 | 4    |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30992

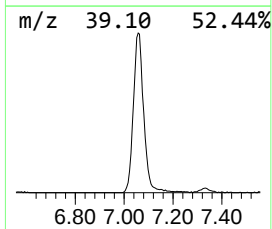
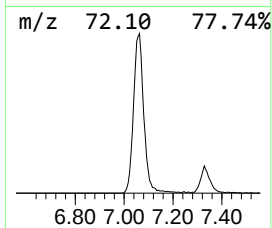
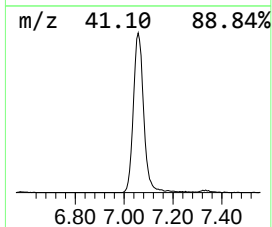
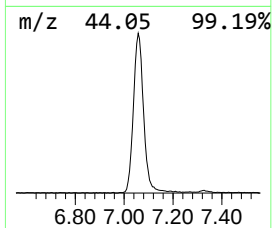
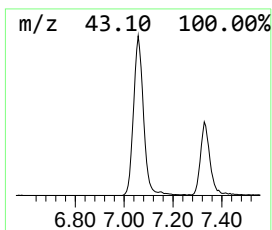
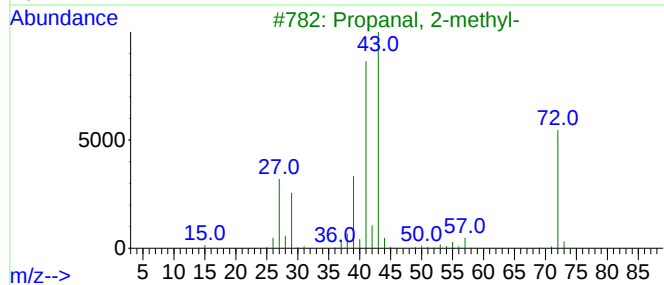
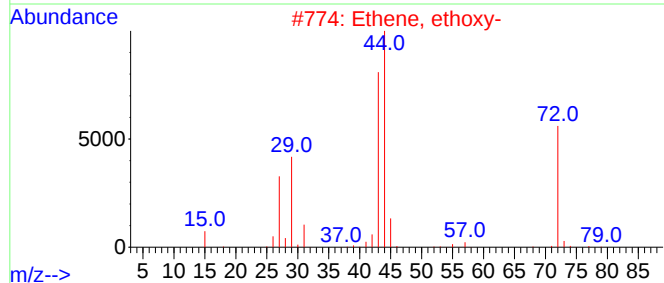
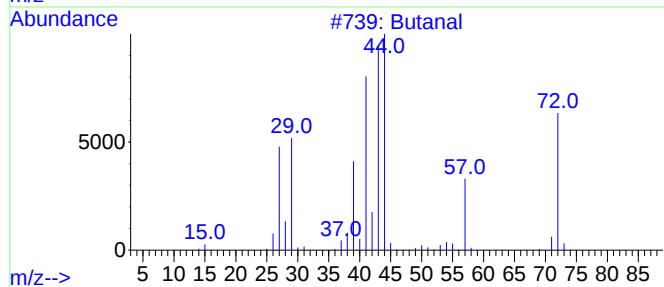
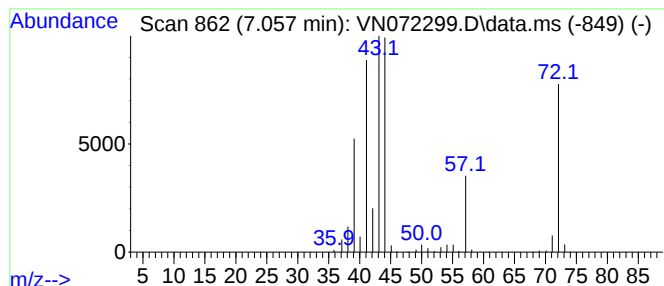
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

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

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Peak Number 3 Butanal Concentration Rank 2

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 7.057 | 106.49 ug/l | 1467420 | Pentafluorobenzene | 8.081 |

| Hit# | of | 5 | Tentative ID           | MW | MolForm | CAS#        | Qual |
|------|----|---|------------------------|----|---------|-------------|------|
| 1    |    |   | Butanal                | 72 | C4H8O   | 000123-72-8 | 94   |
| 2    |    |   | Ethene, ethoxy-        | 72 | C4H8O   | 000109-92-2 | 52   |
| 3    |    |   | Propanal, 2-methyl-    | 72 | C4H8O   | 000078-84-2 | 46   |
| 4    |    |   | 2-Propanone, hydrazone | 72 | C3H8N2  | 005281-20-9 | 38   |
| 5    |    |   | 1-Propene, 3-methoxy-  | 72 | C4H8O   | 000627-40-7 | 32   |



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Sample : N2653-08  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

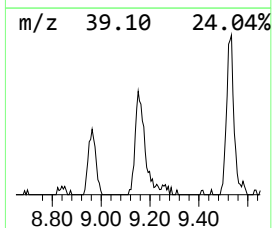
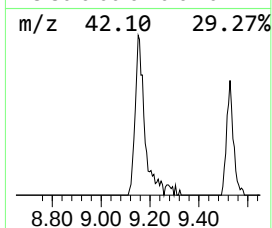
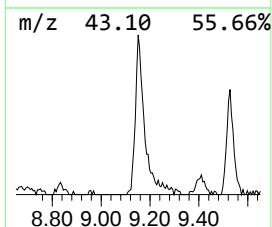
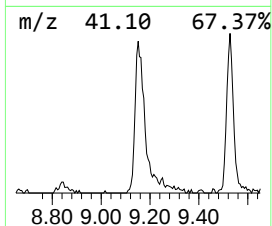
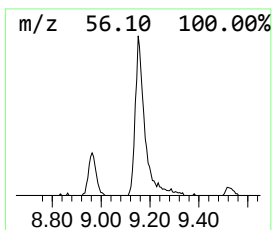
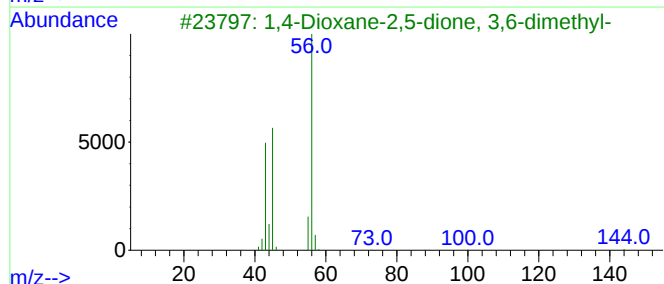
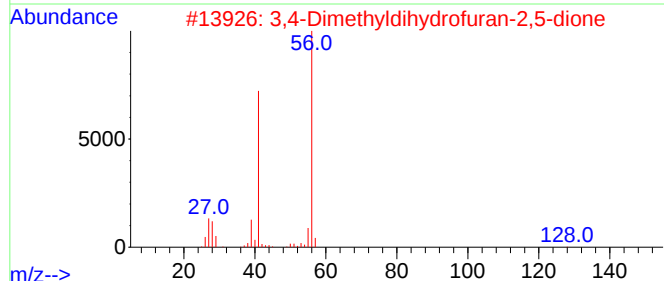
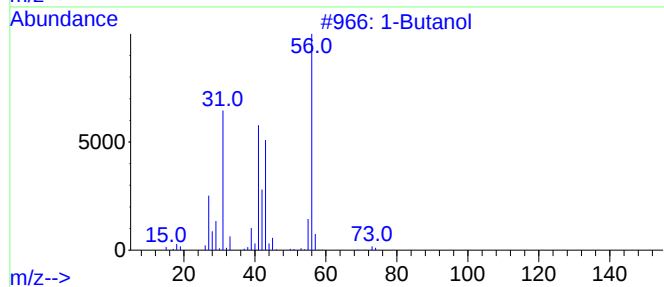
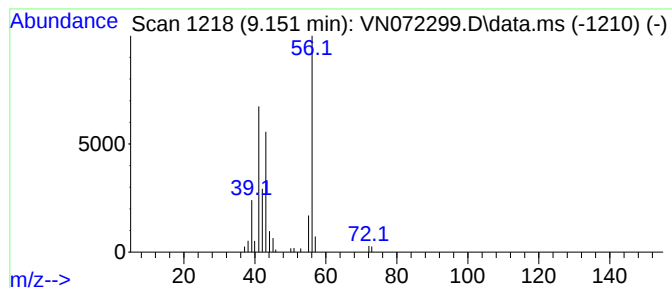
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 1-Butanol Concentration Rank 6

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 9.151 | 8.60 ug/l | 144707 | 1,4-Difluorobenzene | 8.963 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 1-Butanol                           | 74  | C4H10O  | 000071-36-3 | 78   |
| 2    |    |   | 3,4-Dimethyldihydrofuran-2,5-dione  | 128 | C6H8O3  | 007475-92-5 | 40   |
| 3    |    |   | 1,4-Dioxane-2,5-dione, 3,6-dimet... | 144 | C6H8O4  | 000095-96-5 | 38   |
| 4    |    |   | Propane, 2-cyclopropyl-             | 84  | C6H12   | 003638-35-5 | 36   |
| 5    |    |   | Butane, 1-chloro-                   | 92  | C4H9Cl  | 000109-69-3 | 33   |



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ClientSampleId :  
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

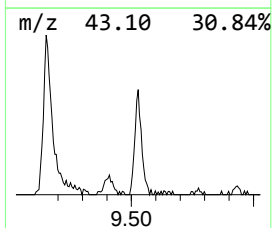
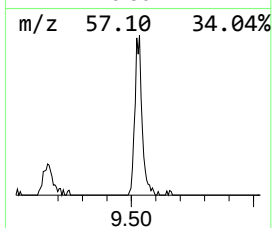
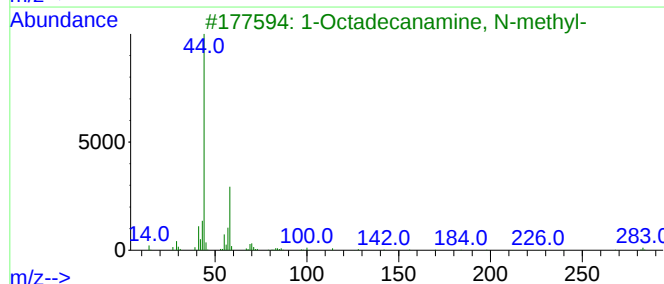
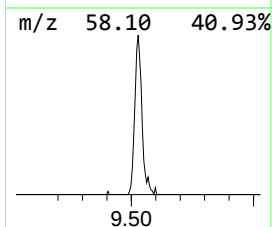
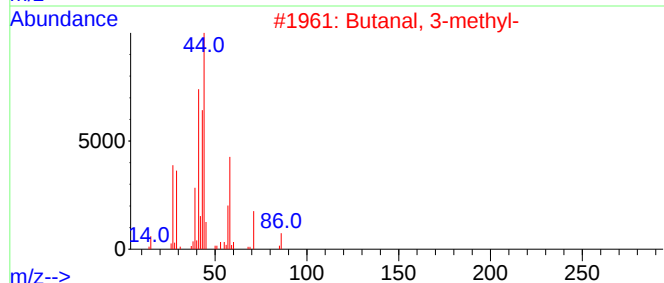
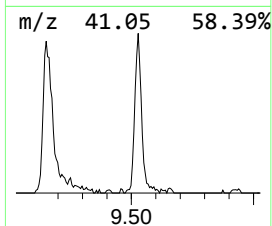
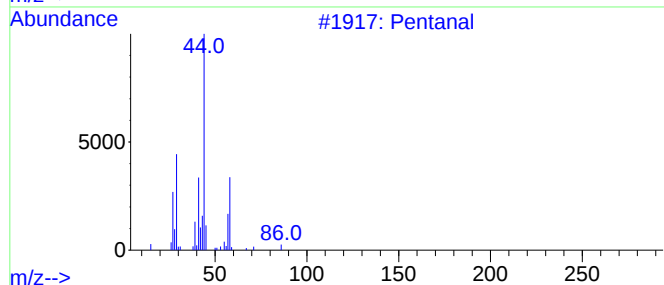
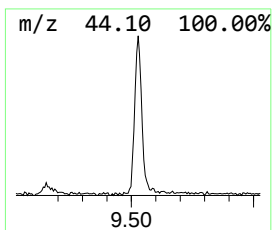
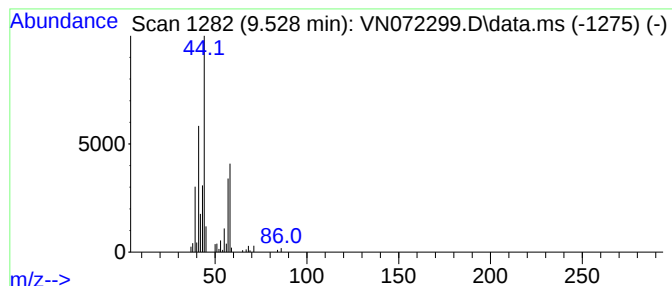
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Pentanal Concentration Rank 5

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 9.528 | 8.68 ug/l | 145907 | 1,4-Difluorobenzene | 8.963 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentanal                    | 86  | C5H10O  | 000110-62-3 | 83   |
| 2    |    |   | Butanal, 3-methyl-          | 86  | C5H10O  | 000590-86-3 | 64   |
| 3    |    |   | 1-Octadecanamine, N-methyl- | 283 | C19H41N | 002439-55-6 | 43   |
| 4    |    |   | Cyclopropyl carbinol        | 72  | C4H8O   | 002516-33-8 | 40   |
| 5    |    |   | Ethanol, 2-(2-propenyloxy)- | 102 | C5H10O2 | 000111-45-5 | 16   |



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

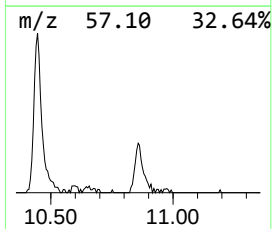
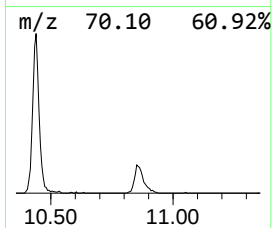
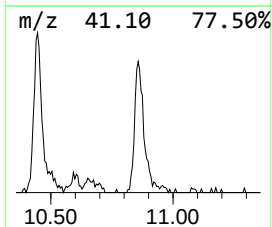
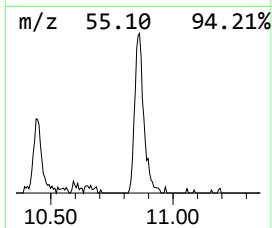
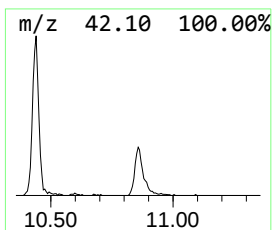
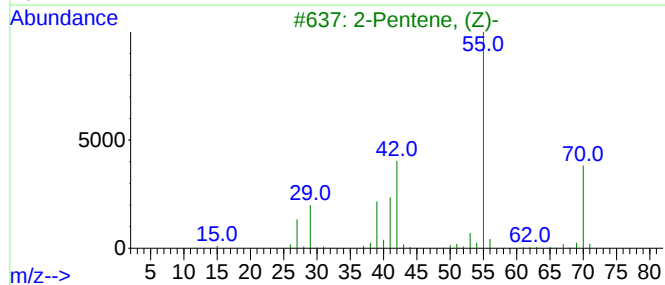
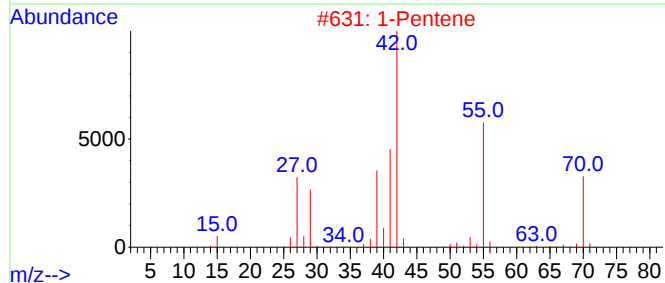
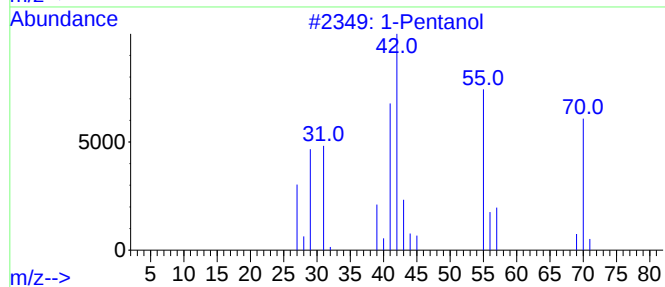
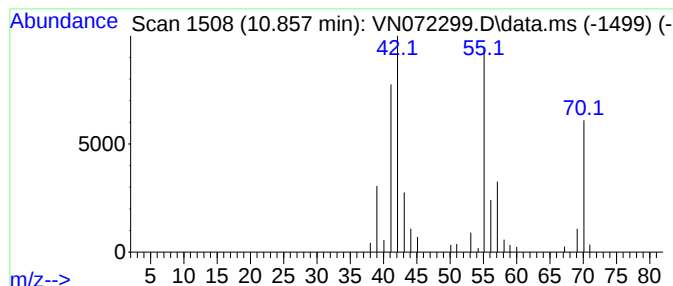
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 1-Pentanol Concentration Rank 8

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 10.857 | 5.51 ug/l | 115218 | Chlorobenzene-d5 | 11.739 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | 1-Pentanol                  | 88  | C5H12O  | 000071-41-0 | 78   |
| 2    |    |   | 1-Pentene                   | 70  | C5H10   | 000109-67-1 | 72   |
| 3    |    |   | 2-Pentene, (Z)-             | 70  | C5H10   | 000627-20-3 | 53   |
| 4    |    |   | Cyclopropane, 1,1-dimethyl- | 70  | C5H10   | 001630-94-0 | 47   |
| 5    |    |   | Pentane, 1-chloro-          | 106 | C5H11Cl | 000543-59-9 | 45   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN050222\  
Data File : VN072299.D  
Acq On : 02 May 2022 17:11  
Operator : JC\MD  
Sample : N2653-08  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30992

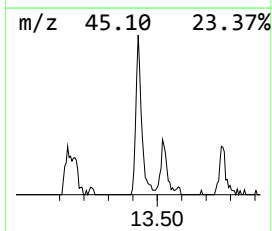
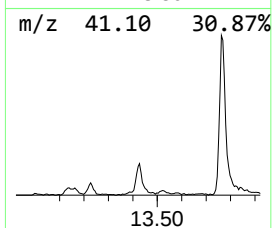
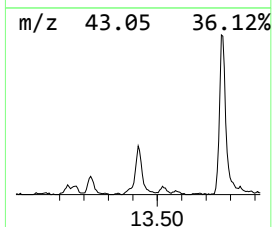
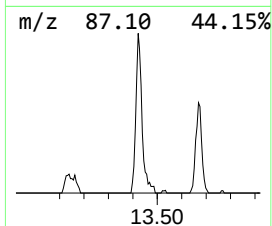
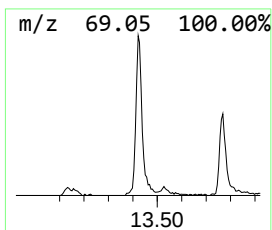
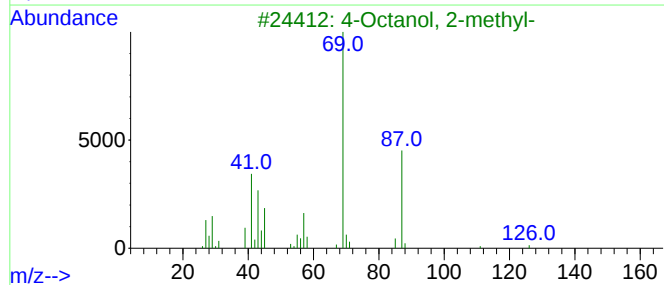
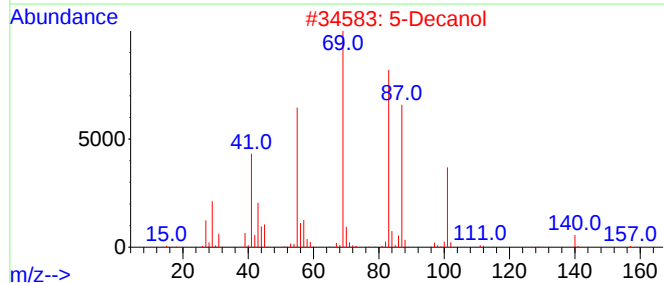
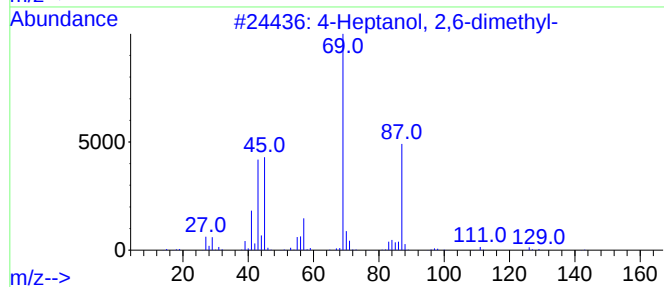
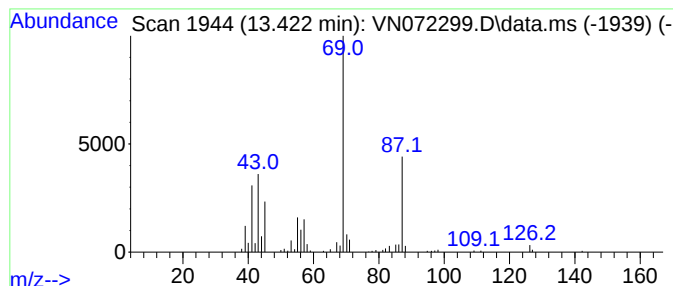
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Quant Title : SW846 8260

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

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Peak Number 7 4-Heptanol, 2,6-dimethyl- Concentration Rank 4

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.422 | 13.38 ug/l | 189135 | 1,4-Dichlorobenzene-d4 | 13.669 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Heptanol, 2,6-dimethyl- | 144 | C9H20O  | 000108-82-7 | 78   |
| 2    |    |   | 5-Decanol                 | 158 | C10H22O | 005205-34-5 | 72   |
| 3    |    |   | 4-Octanol, 2-methyl-      | 144 | C9H20O  | 040575-41-5 | 64   |
| 4    |    |   | 5-Nonanol                 | 144 | C9H20O  | 000623-93-8 | 64   |
| 5    |    |   | 1-Octyn-4-ol              | 126 | C8H14O  | 052517-92-7 | 59   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN050222\  
Data File : VN072299.D  
Acq On : 02 May 2022 17:11  
Operator : JC\MD  
Sample : N2653-08  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30992

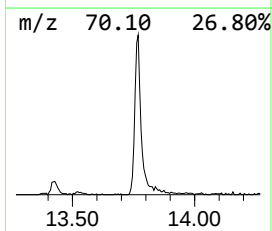
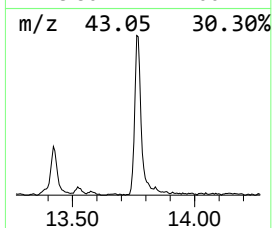
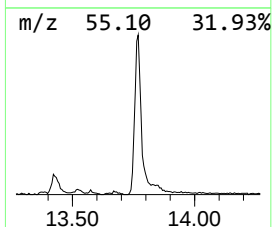
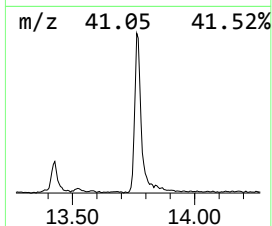
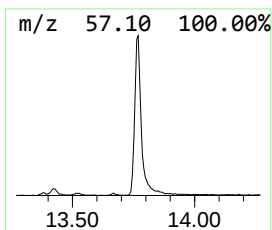
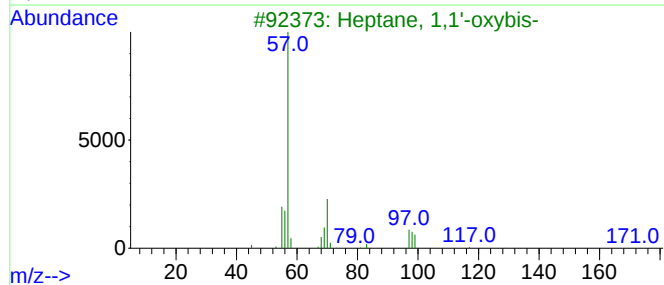
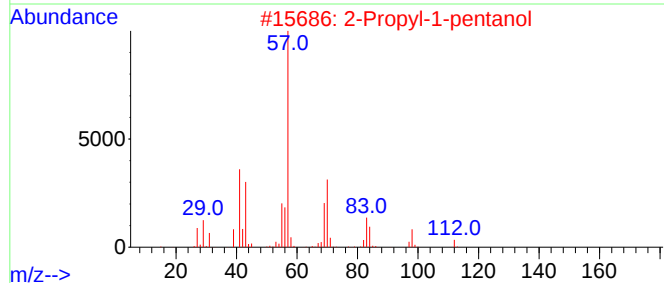
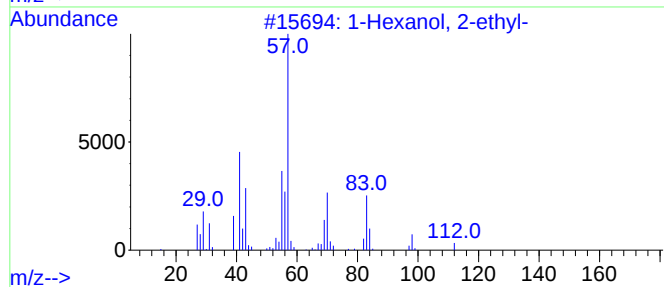
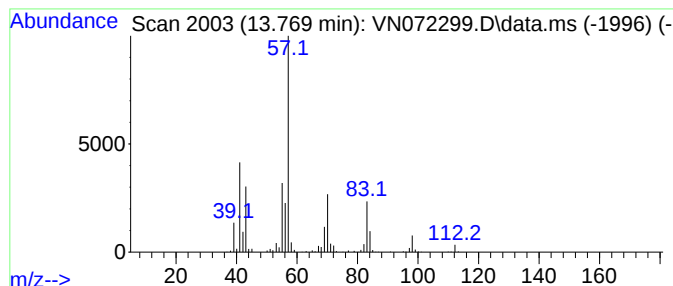
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Quant Title : SW846 8260

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

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Peak Number 8 1-Hexanol, 2-ethyl- Concentration Rank 3

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 13.769 | 59.54 ug/l | 841516 | 1,4-Dichlorobenzene-d4 | 13.669 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | 1-Hexanol, 2-ethyl-                 | 130 | C8H18O      | 000104-76-7  | 90   |
| 2    |    |   | 2-Propyl-1-pentanol                 | 130 | C8H18O      | 058175-57-8  | 53   |
| 3    |    |   | Heptane, 1,1'-oxybis-               | 214 | C14H30O     | 000629-64-1  | 53   |
| 4    |    |   | Heptyl isobutyl carbonate           | 216 | C12H24O3    | 959068-08-7  | 50   |
| 5    |    |   | Pentadecafluorooctanoic acid, 2-... | 526 | C16H17F15O2 | 1000406-80-9 | 45   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN050222\  
Data File : VN072299.D  
Acq On : 02 May 2022 17:11  
Operator : JC\MD  
Sample : N2653-08  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
30992

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N042622W.M  
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Ethanol            | 3.681  | 114.4   | ug/l  | 1576520  | 1                     | 8.081  | 688981  | 50.0 |
| Butanal            | 7.057  | 106.5   | ug/l  | 1467420  | 1                     | 8.081  | 688981  | 50.0 |
| 1-Butanol          | 9.151  | 8.6     | ug/l  | 144707   | 2                     | 8.963  | 840901  | 50.0 |
| Pentanal           | 9.528  | 8.7     | ug/l  | 145907   | 2                     | 8.963  | 840901  | 50.0 |
| 1-Pentanol         | 10.857 | 5.5     | ug/l  | 115218   | 3                     | 11.739 | 1046300 | 50.0 |
| 4-Heptanol, 2,6... | 13.422 | 13.4    | ug/l  | 189135   | 4                     | 13.669 | 706649  | 50.0 |
| 1-Hexanol, 2-et... | 13.769 | 59.5    | ug/l  | 841516   | 4                     | 13.669 | 706649  | 50.0 |