

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN060523\  
 Data File : VN078052.D  
 Acq On : 05 Jun 2023 18:21  
 Operator : JC\MD  
 Sample : 03018-04  
 Misc : 5.0mL/MSVOA\_N/WATER  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 362

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\82N051523W.M  
 Title : SW846 8260

Signal : TIC: VN078052.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         | 2.089       | 20            | 23          | 34           | rVB3     | 15929          | 26040         | 1.16%           | 0.157%        |
| 2         | 2.836       | 138           | 150         | 154          | rBV4     | 32718          | 85303         | 3.79%           | 0.516%        |
| 3         | 4.442       | 415           | 423         | 425          | rBV      | 13217          | 25081         | 1.11%           | 0.152%        |
| 4         | 5.277       | 555           | 565         | 566          | rBV2     | 14706          | 24527         | 1.09%           | 0.148%        |
| 5         | 7.577       | 947           | 956         | 963          | rBV4     | 21637          | 53105         | 2.36%           | 0.321%        |
| 6         | 8.177       | 1048          | 1058        | 1062         | rBV      | 308998         | 739813        | 32.89%          | 4.474%        |
| 7         | 8.235       | 1062          | 1068        | 1081         | rVB      | 527183         | 1177275       | 52.34%          | 7.119%        |
| 8         | 8.588       | 1113          | 1128        | 1136         | rBV      | 318232         | 745268        | 33.13%          | 4.507%        |
| 9         | 8.700       | 1136          | 1147        | 1153         | rBV2     | 175558         | 505320        | 22.46%          | 3.056%        |
| 10        | 9.106       | 1207          | 1216        | 1226         | rBV      | 788762         | 1628905       | 72.41%          | 9.850%        |
| 11        | 9.677       | 1305          | 1313        | 1319         | rBV2     | 86504          | 194045        | 8.63%           | 1.173%        |
| 12        | 9.747       | 1319          | 1325        | 1338         | rVB      | 598980         | 1107651       | 49.24%          | 6.698%        |
| 13        | 10.365      | 1423          | 1430        | 1439         | rBV      | 316485         | 547593        | 24.34%          | 3.311%        |
| 14        | 10.571      | 1458          | 1465        | 1474         | rBV      | 1182153        | 2249461       | 100.00%         | 13.603%       |
| 15        | 10.735      | 1487          | 1493        | 1502         | rVB      | 109448         | 194498        | 8.65%           | 1.176%        |
| 16        | 10.994      | 1530          | 1537        | 1545         | rBV      | 384479         | 645590        | 28.70%          | 3.904%        |
| 17        | 11.088      | 1545          | 1553        | 1561         | rVV3     | 53061          | 105387        | 4.68%           | 0.637%        |
| 18        | 11.176      | 1561          | 1568        | 1570         | rVV      | 203129         | 329186        | 14.63%          | 1.991%        |
| 19        | 11.206      | 1570          | 1573        | 1583         | rVV      | 279963         | 471058        | 20.94%          | 2.849%        |
| 20        | 11.294      | 1583          | 1588        | 1595         | rVB      | 59164          | 101314        | 4.50%           | 0.613%        |
| 21        | 11.606      | 1633          | 1641        | 1652         | rBV2     | 621033         | 974893        | 43.34%          | 5.895%        |
| 22        | 11.776      | 1664          | 1670        | 1676         | rVB5     | 12985          | 24577         | 1.09%           | 0.149%        |
| 23        | 11.871      | 1678          | 1686        | 1697         | rVB      | 1035986        | 1901595       | 84.54%          | 11.499%       |
| 24        | 12.312      | 1755          | 1761        | 1767         | rBV5     | 17428          | 31104         | 1.38%           | 0.188%        |
| 25        | 12.853      | 1845          | 1853        | 1864         | rBV      | 787332         | 1376790       | 61.21%          | 8.326%        |
| 26        | 13.800      | 2005          | 2014        | 2020         | rBV      | 727269         | 1232738       | 54.80%          | 7.455%        |
| 27        | 13.859      | 2020          | 2024        | 2030         | rVB4     | 22953          | 38629         | 1.72%           | 0.234%        |

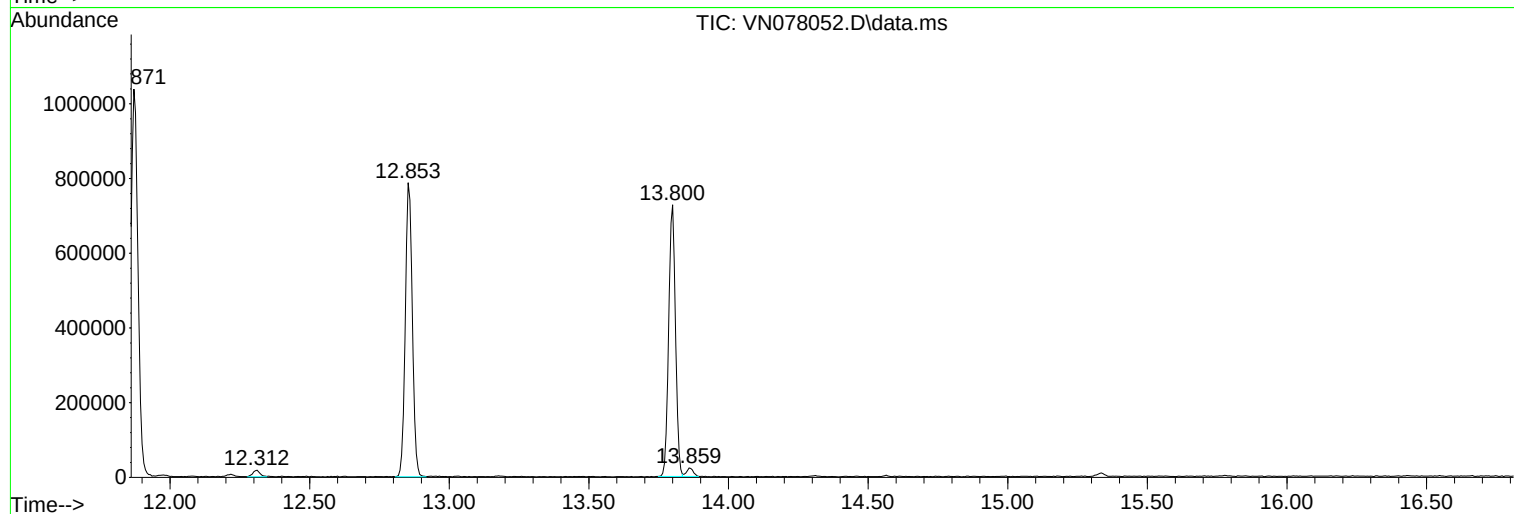
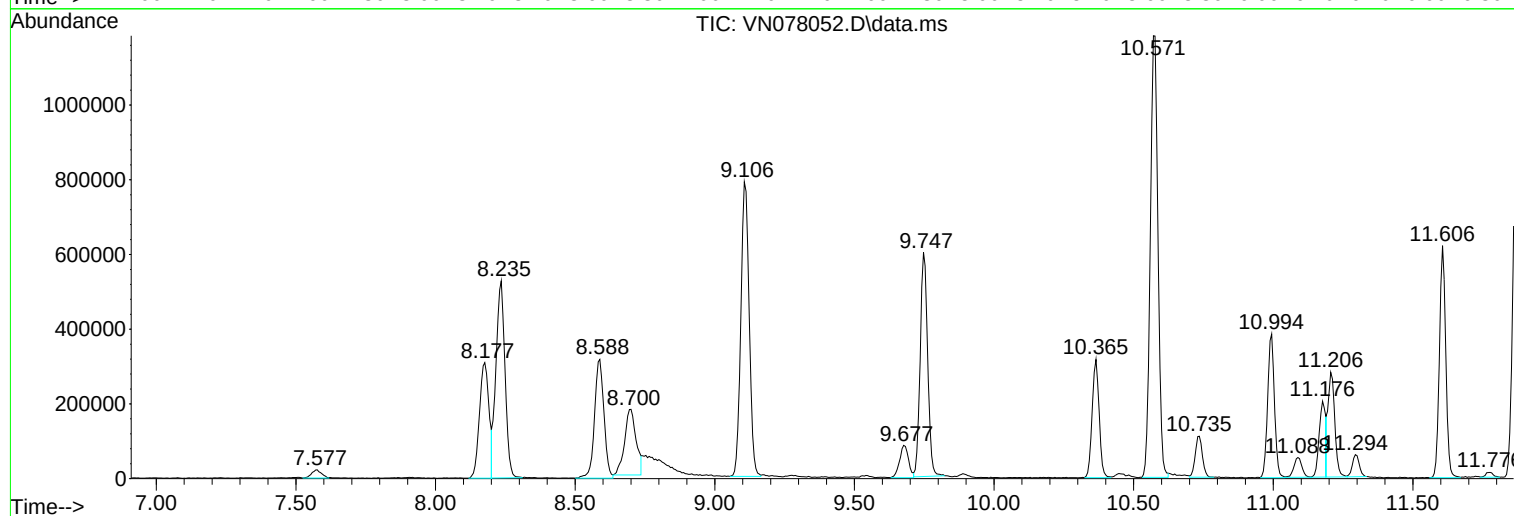
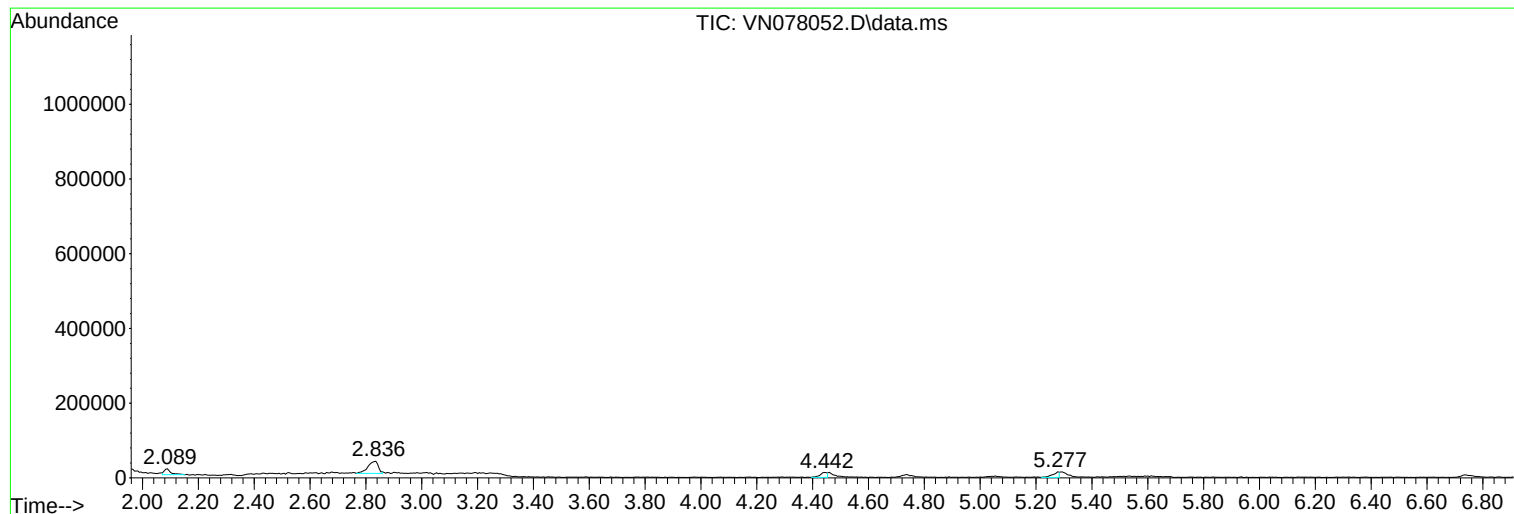
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.M  
Quant Title : SW846 8260

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



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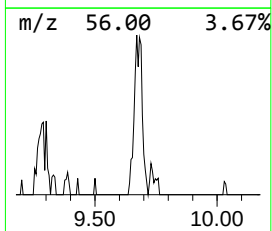
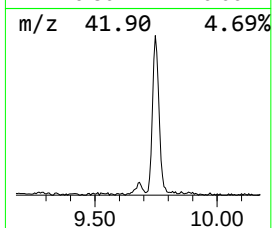
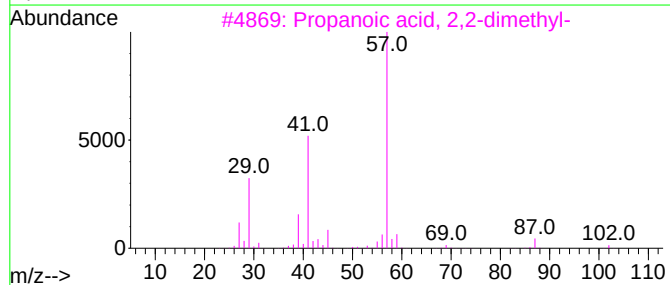
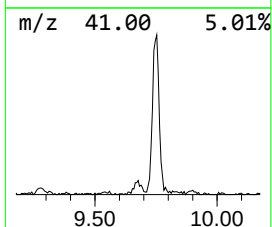
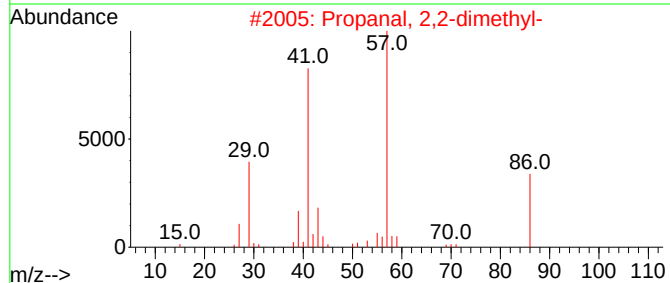
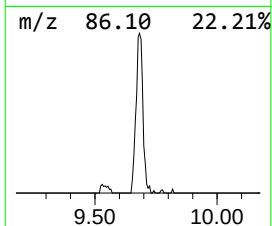
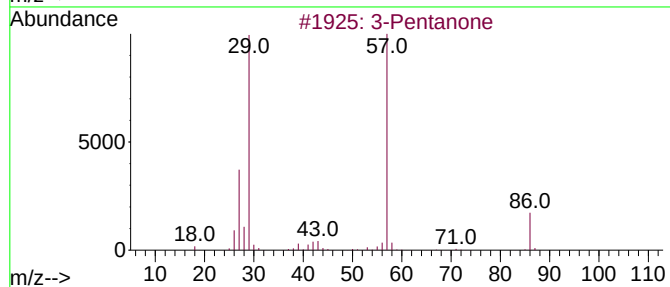
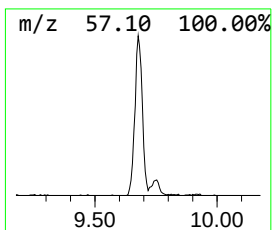
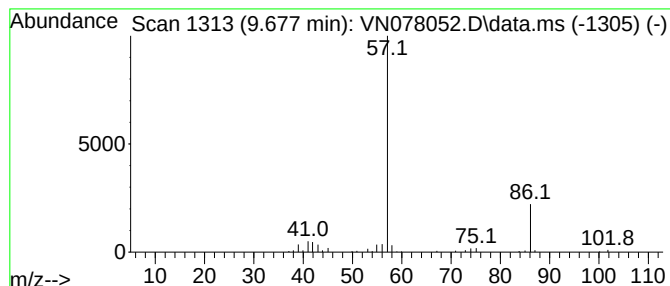
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 3-Pentanone Concentration Rank 7

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 9.677 | 5.96 ug/l | 194045 | 1,4-Difluorobenzene | 9.106 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Pentanone                   | 86  | C5H10O  | 000096-22-0 | 64   |
| 2    |    |   | Propanal, 2,2-dimethyl-       | 86  | C5H10O  | 000630-19-3 | 40   |
| 3    |    |   | Propanoic acid, 2,2-dimethyl- | 102 | C5H10O2 | 000075-98-9 | 9    |
| 4    |    |   | Ethyl-1-propenyl ether        | 86  | C5H10O  | 000928-55-2 | 9    |
| 5    |    |   | Butanoic acid, 2-oxo-         | 102 | C4H6O3  | 000600-18-0 | 9    |



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ClientSampleId :  
362

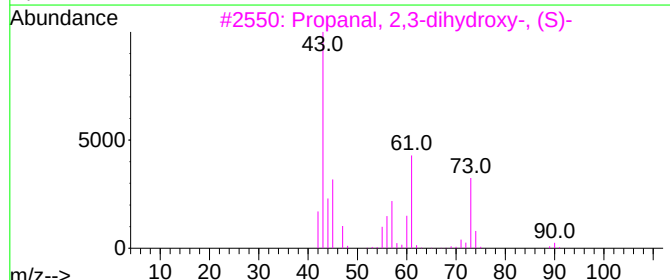
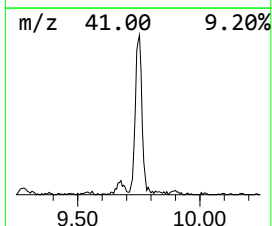
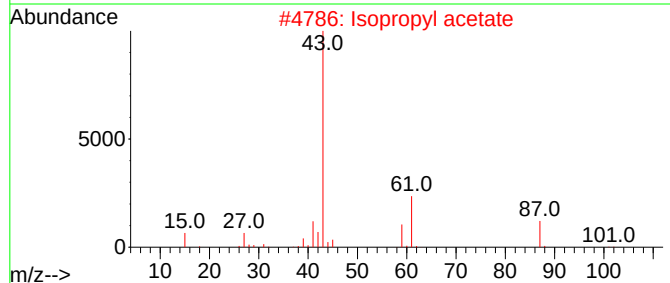
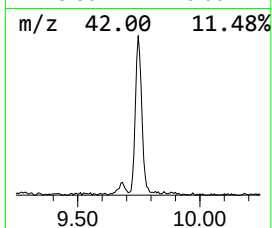
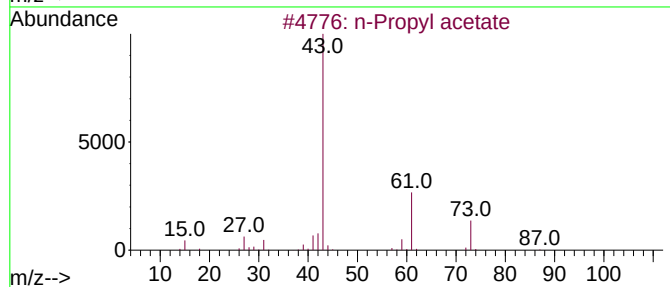
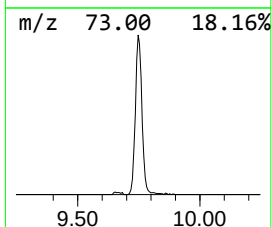
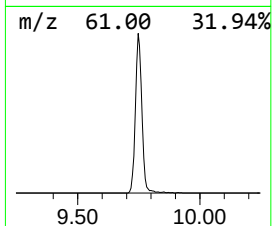
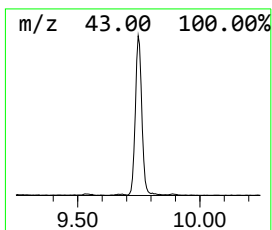
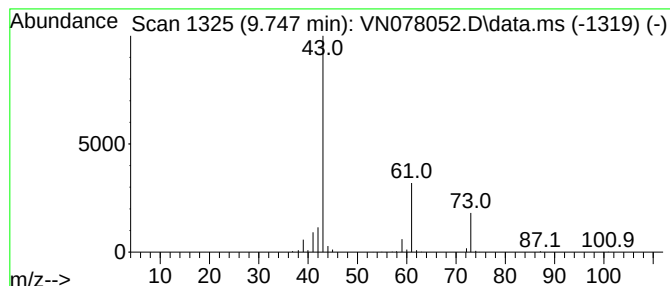
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.M  
Quant Title : SW846 8260

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

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Peak Number 2 n-Propyl acetate Concentration Rank 1

| R.T.  | EstConc    | Area    | Relative to ISTD    | R.T.  |
|-------|------------|---------|---------------------|-------|
| 9.747 | 34.00 ug/l | 1107650 | 1,4-Difluorobenzene | 9.106 |

| Hit# | of | 5 | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|-----|---------|-------------|------|
| 1    |    |   | n-Propyl acetate               | 102 | C5H10O2 | 000109-60-4 | 83   |
| 2    |    |   | Isopropyl acetate              | 102 | C5H10O2 | 000108-21-4 | 36   |
| 3    |    |   | Propanal, 2,3-dihydroxy-, (S)- | 90  | C3H6O3  | 000497-09-6 | 36   |
| 4    |    |   | Isobutylamine                  | 73  | C4H11N  | 000078-81-9 | 9    |
| 5    |    |   | 1-Butanamine                   | 73  | C4H11N  | 000109-73-9 | 7    |



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ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.M  
Quant Title : SW846 8260

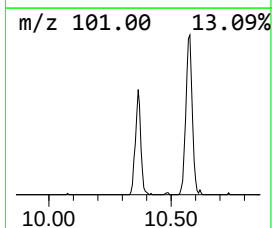
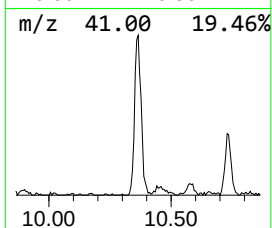
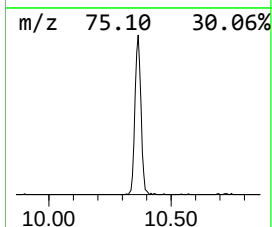
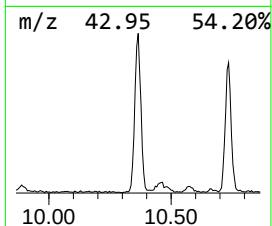
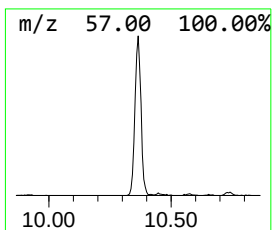
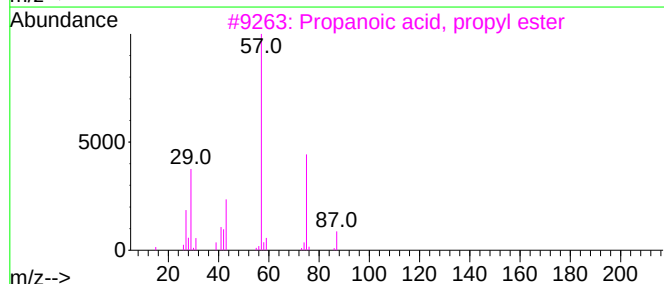
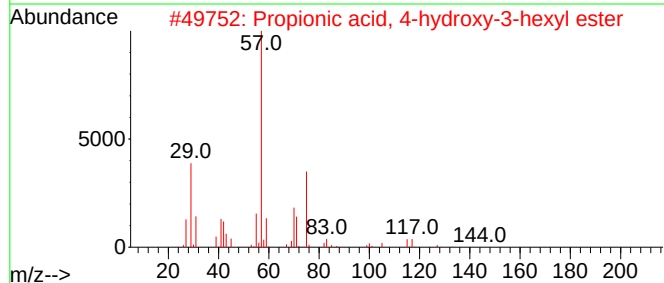
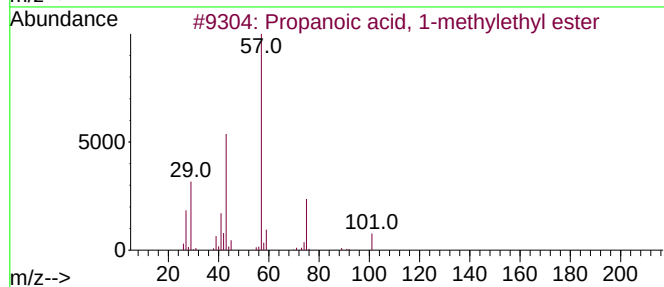
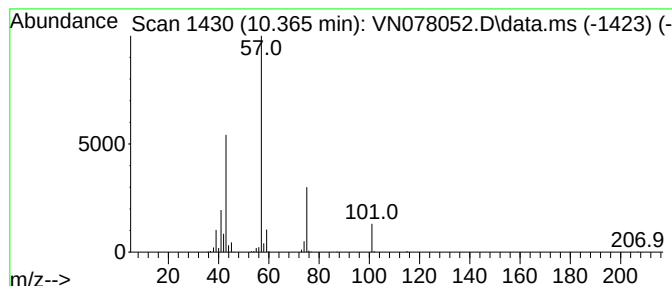
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Propanoic acid, 1-methyleth... Concentration Rank 4

| R.T.   | EstConc    | Area   | Relative to ISTD    | R.T.  |
|--------|------------|--------|---------------------|-------|
| 10.365 | 16.81 ug/l | 547593 | 1,4-Difluorobenzene | 9.106 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Propanoic acid, 1-methylethyl ester | 116 | C6H12O2  | 000637-78-5  | 83   |
| 2    |    |   | Propionic acid, 4-hydroxy-3-hexy... | 174 | C9H18O3  | 1000151-16-9 | 42   |
| 3    |    |   | Propanoic acid, propyl ester        | 116 | C6H12O2  | 000106-36-5  | 33   |
| 4    |    |   | di-tert-Butyl dicarbonate           | 218 | C10H18O5 | 024424-99-5  | 10   |
| 5    |    |   | 1-Propanol, 2-methyl-               | 74  | C4H10O   | 000078-83-1  | 9    |



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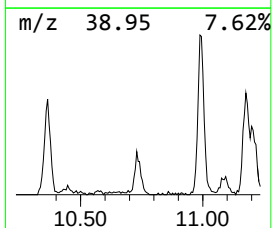
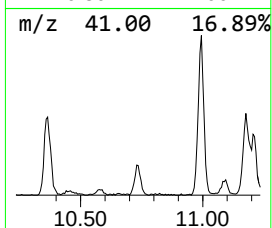
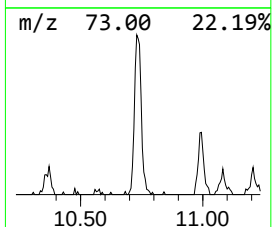
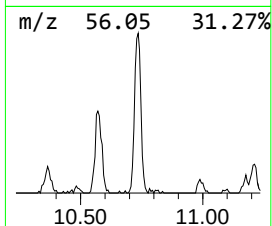
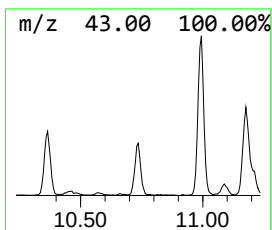
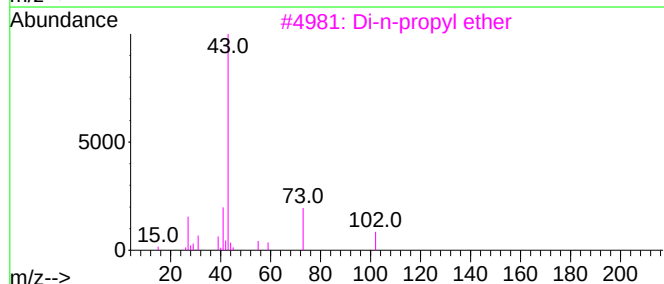
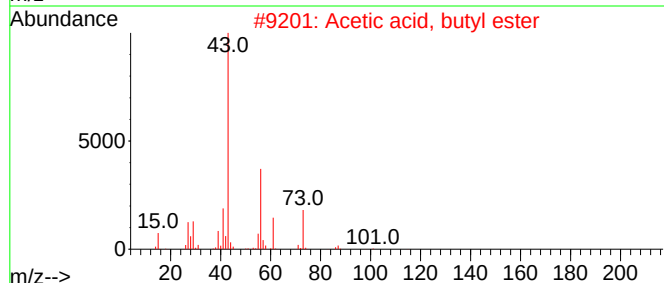
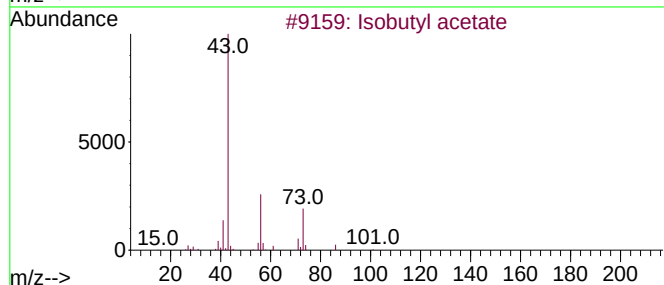
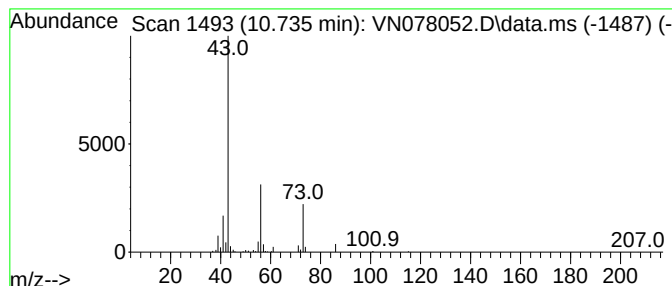
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Peak Number 4 Isobutyl acetate Concentration Rank 8

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 10.735 | 5.11 ug/l | 194498 | Chlorobenzene-d5 | 11.871 |

| Hit# | of | 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|----|---|--------------------------|-----|---------|-------------|------|
| 1    |    |   | Isobutyl acetate         | 116 | C6H12O2 | 000110-19-0 | 78   |
| 2    |    |   | Acetic acid, butyl ester | 116 | C6H12O2 | 000123-86-4 | 36   |
| 3    |    |   | Di-n-propyl ether        | 102 | C6H14O  | 000111-43-3 | 32   |
| 4    |    |   | Pentanoic acid, 4-oxo-   | 116 | C5H8O3  | 000123-76-2 | 28   |
| 5    |    |   | 2-Butanone, 3-methyl-    | 86  | C5H10O  | 000563-80-4 | 14   |



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Quant Title : SW846 8260

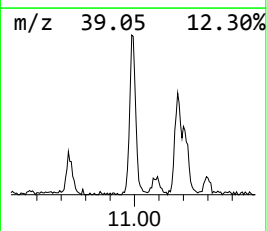
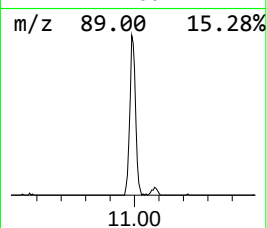
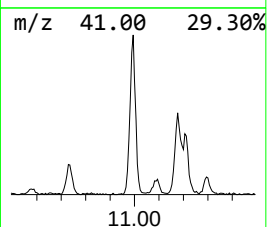
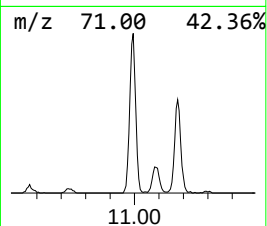
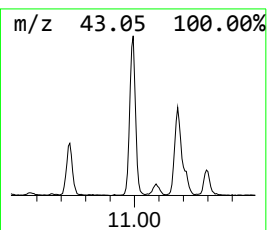
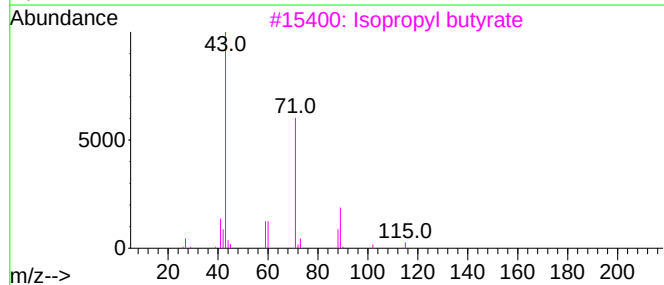
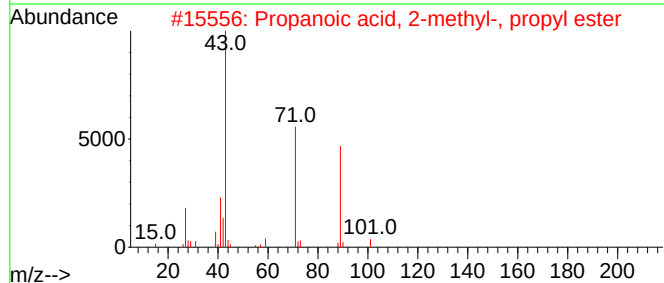
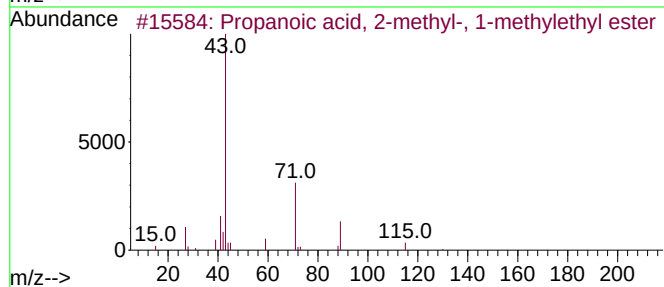
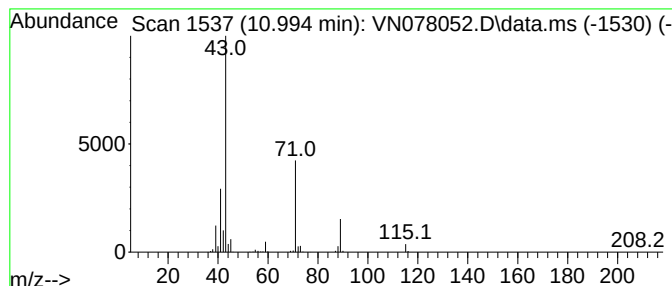
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Propanoic acid, 2-methyl-, ... Concentration Rank 3

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 10.994 | 16.98 ug/l | 645590 | Chlorobenzene-d5 | 11.871 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2 | 000617-50-5 | 83   |
| 2    |    |   | Propanoic acid, 2-methyl-, propy... | 130 | C7H14O2 | 000644-49-5 | 78   |
| 3    |    |   | Isopropyl butyrate                  | 130 | C7H14O2 | 000638-11-9 | 64   |
| 4    |    |   | 2-Oxo-n-valeric acid                | 116 | C5H8O3  | 001821-02-9 | 47   |
| 5    |    |   | 2,3-Hexanedione                     | 114 | C6H10O2 | 003848-24-6 | 42   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN060523\  
Data File : VN078052.D  
Acq On : 05 Jun 2023 18:21  
Operator : JC\MD  
Sample : 03018-04  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
362

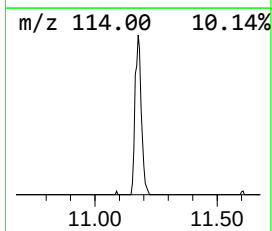
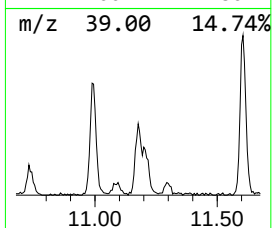
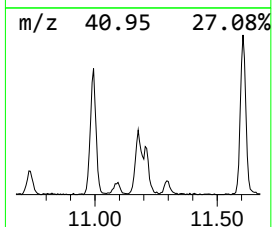
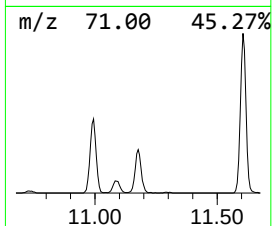
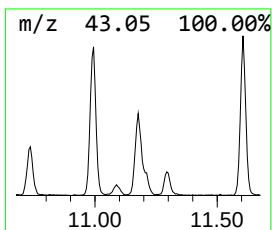
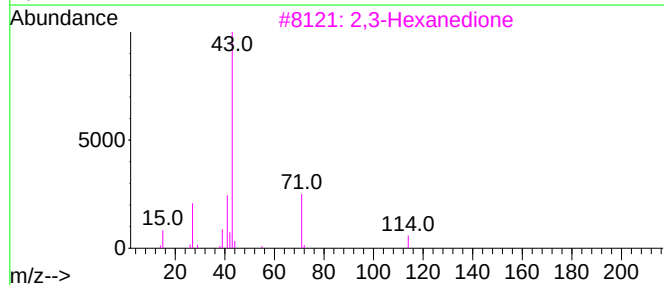
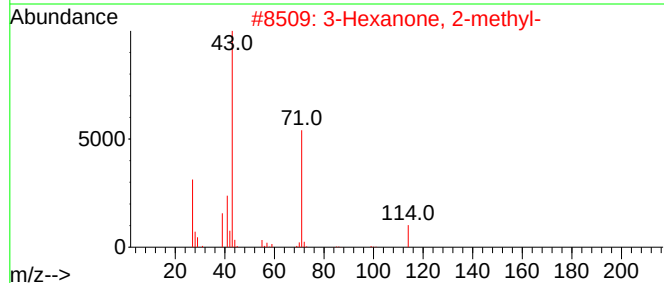
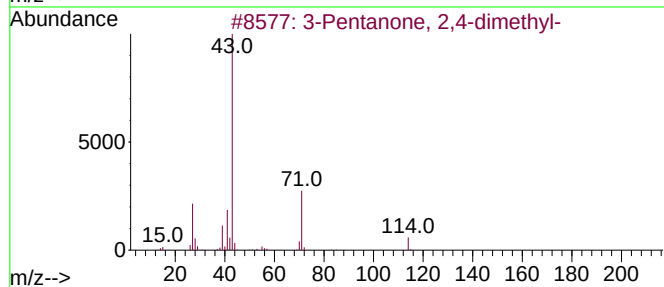
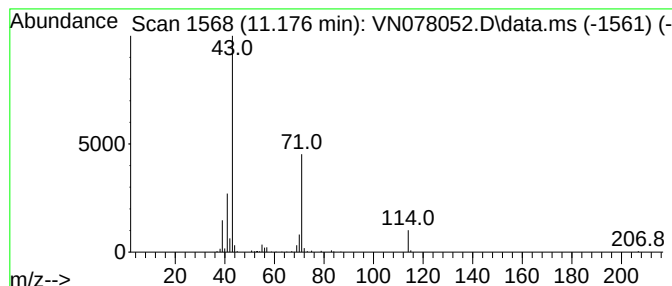
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Quant Title : SW846 8260

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

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Peak Number 6 3-Pentanone, 2,4-dimethyl- Concentration Rank 6

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 11.177 | 8.66 ug/l | 329186 | Chlorobenzene-d5 | 11.871 |

| Hit# | of | 5 | Tentative ID               | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------|-----|---------|-------------|------|
| 1    |    |   | 3-Pentanone, 2,4-dimethyl- | 114 | C7H14O  | 000565-80-0 | 86   |
| 2    |    |   | 3-Hexanone, 2-methyl-      | 114 | C7H14O  | 007379-12-6 | 86   |
| 3    |    |   | 2,3-Hexanedione            | 114 | C6H10O2 | 003848-24-6 | 72   |
| 4    |    |   | 4-Heptanone                | 114 | C7H14O  | 000123-19-3 | 59   |
| 5    |    |   | Pyrrolidine                | 71  | C4H9N   | 000123-75-1 | 50   |





Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN060523\  
Data File : VN078052.D  
Acq On : 05 Jun 2023 18:21  
Operator : JC\MD  
Sample : 03018-04  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.M  
Quant Title : SW846 8260

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

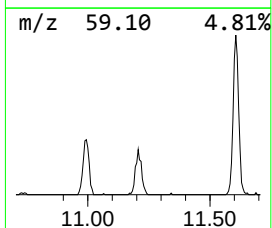
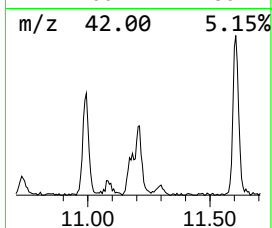
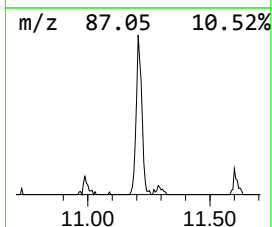
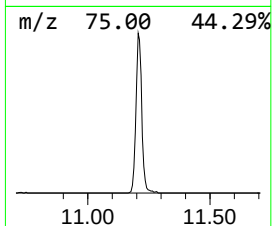
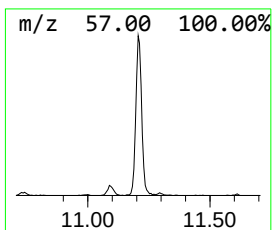
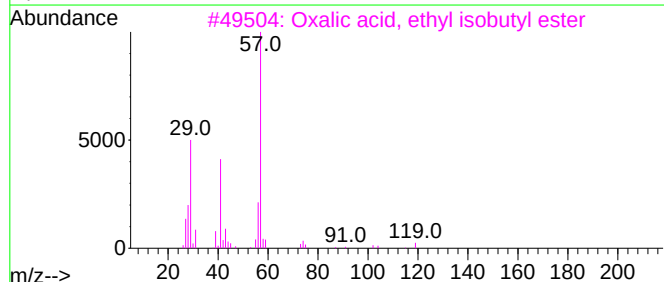
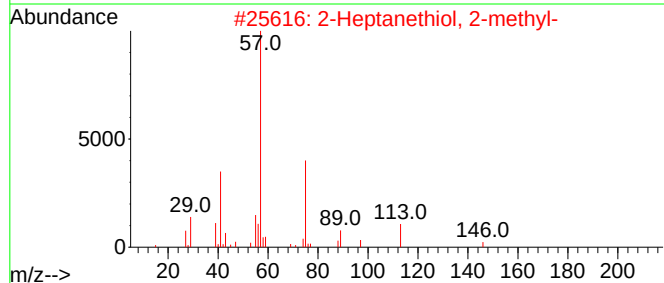
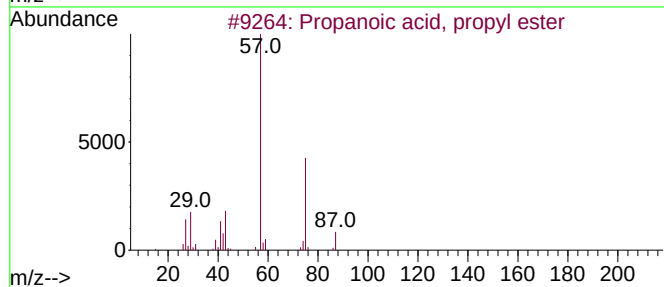
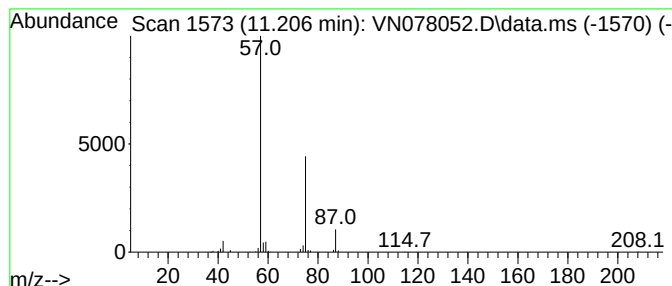
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Peak Number 7 Propanoic acid, propyl ester Concentration Rank 5

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 11.206 | 12.39 ug/l | 471058 | Chlorobenzene-d5 | 11.871 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm | CAS#         | Qual |
|------|----|---|-----------------------------------|-----|---------|--------------|------|
| 1    |    |   | Propanoic acid, propyl ester      | 116 | C6H12O2 | 000106-36-5  | 83   |
| 2    |    |   | 2-Heptanethiol, 2-methyl-         | 146 | C8H18S  | 000763-20-2  | 9    |
| 3    |    |   | Oxalic acid, ethyl isobutyl ester | 174 | C8H14O4 | 1000309-36-7 | 9    |
| 4    |    |   | Isobutyl ether                    | 130 | C8H18O  | 000628-55-7  | 9    |
| 5    |    |   | Propanoic acid, butyl ester       | 130 | C7H14O2 | 000590-01-2  | 9    |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN060523\  
Data File : VN078052.D  
Acq On : 05 Jun 2023 18:21  
Operator : JC\MD  
Sample : 03018-04  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.M  
Quant Title : SW846 8260

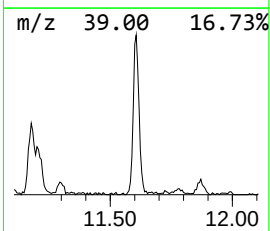
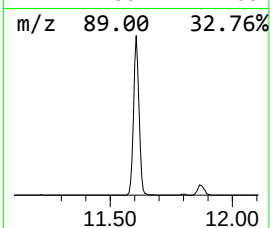
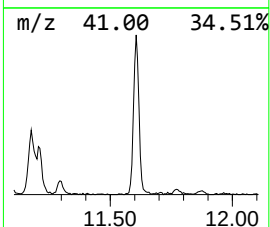
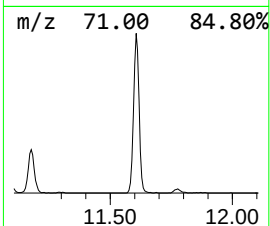
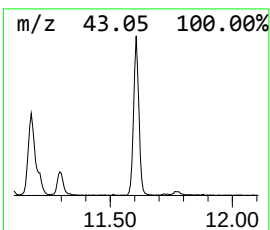
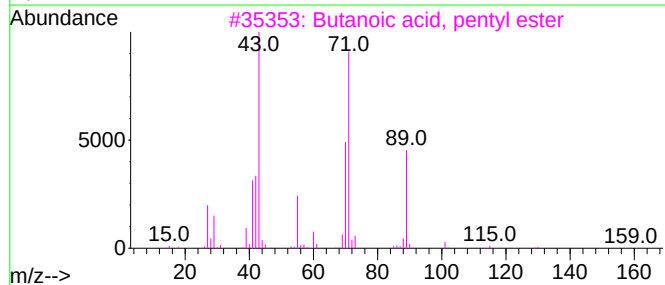
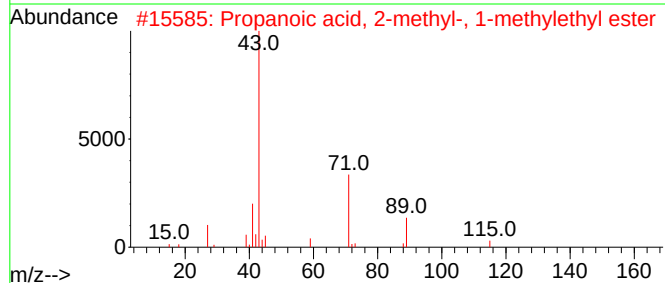
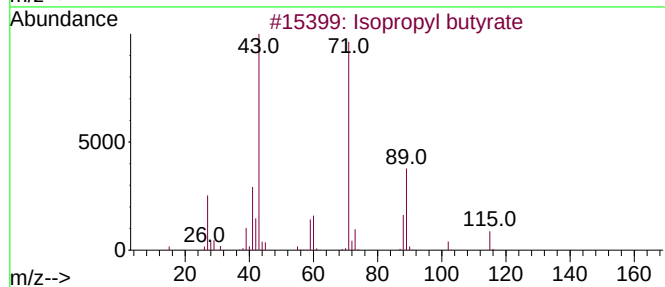
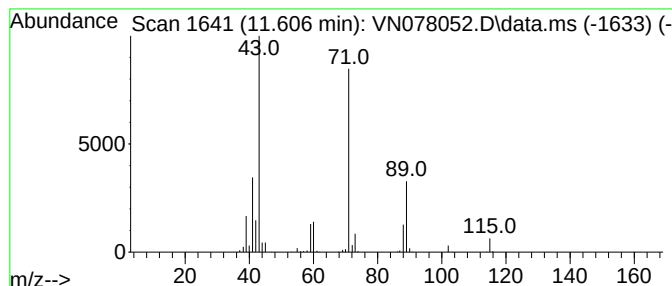
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Isopropyl butyrate Concentration Rank 2

| R.T.   | EstConc    | Area   | Relative to ISTD | R.T.   |
|--------|------------|--------|------------------|--------|
| 11.606 | 25.63 ug/l | 974893 | Chlorobenzene-d5 | 11.871 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Isopropyl butyrate                  | 130 | C7H14O2  | 000638-11-9 | 91   |
| 2    |    |   | Propanoic acid, 2-methyl-, 1-met... | 130 | C7H14O2  | 000617-50-5 | 72   |
| 3    |    |   | Butanoic acid, pentyl ester         | 158 | C9H18O2  | 000540-18-1 | 64   |
| 4    |    |   | Propanoic acid, 2-methyl-, penty... | 158 | C9H18O2  | 002445-72-9 | 64   |
| 5    |    |   | Ethane-1,1-diol dibutanoate         | 202 | C10H18O4 | 025572-25-2 | 50   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_N\Data\VN060523\  
Data File : VN078052.D  
Acq On : 05 Jun 2023 18:21  
Operator : JC\MD  
Sample : 03018-04  
Misc : 5.0mL/MSVOA\_N/WATER  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
362

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_N\methods\82N051523W.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 |
| 3-Pentanone        | 9.677  | 6.0     | ug/l  | 194045   | 2                     | 9.106  | 1628910 | 50.0 |
| n-Propyl acetate   | 9.747  | 34.0    | ug/l  | 1107650  | 2                     | 9.106  | 1628910 | 50.0 |
| Propanoic acid,... | 10.365 | 16.8    | ug/l  | 547593   | 2                     | 9.106  | 1628910 | 50.0 |
| Isobutyl acetate   | 10.735 | 5.1     | ug/l  | 194498   | 3                     | 11.871 | 1901600 | 50.0 |
| Propanoic acid,... | 10.994 | 17.0    | ug/l  | 645590   | 3                     | 11.871 | 1901600 | 50.0 |
| 3-Pentanone, 2,... | 11.177 | 8.7     | ug/l  | 329186   | 3                     | 11.871 | 1901600 | 50.0 |
| Propanoic acid,... | 11.206 | 12.4    | ug/l  | 471058   | 3                     | 11.871 | 1901600 | 50.0 |
| Isopropyl butyrate | 11.606 | 25.6    | ug/l  | 974893   | 3                     | 11.871 | 1901600 | 50.0 |