

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX091923\  
 Data File : VX037806.D  
 Acq On : 19 Sep 2023 15:16  
 Operator : JC/MD  
 Sample : 04479-01  
 Misc : 5.0mL/MSVOA\_X/WATER  
 ALS Vial : 16 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 1026

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\82X091523W.M  
 Title : SW846 8260

Signal : TIC: VX037806.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         | 1.142       | 6             | 9           | 18           | rVB      | 34648          | 36674         | 1.29%           | 0.282%        |
| 2         | 1.453       | 56            | 60          | 69           | rBV      | 44609          | 50019         | 1.76%           | 0.384%        |
| 3         | 2.294       | 193           | 198         | 206          | rVB      | 22832          | 36131         | 1.27%           | 0.277%        |
| 4         | 2.380       | 206           | 212         | 225          | rVV      | 60110          | 100181        | 3.53%           | 0.769%        |
| 5         | 3.331       | 359           | 368         | 379          | rBV      | 17941          | 41645         | 1.47%           | 0.320%        |
| 6         | 4.233       | 505           | 516         | 537          | rBV      | 1062427        | 2841442       | 100.00%         | 21.821%       |
| 7         | 4.556       | 559           | 569         | 586          | rBV      | 306490         | 847968        | 29.84%          | 6.512%        |
| 8         | 4.995       | 631           | 641         | 656          | rBV2     | 29682          | 101783        | 3.58%           | 0.782%        |
| 9         | 5.391       | 693           | 706         | 722          | rBV      | 136290         | 394384        | 13.88%          | 3.029%        |
| 10        | 5.556       | 722           | 733         | 749          | rVV      | 235222         | 661838        | 23.29%          | 5.083%        |
| 11        | 5.958       | 784           | 799         | 809          | rBV2     | 149965         | 387739        | 13.65%          | 2.978%        |
| 12        | 6.111       | 818           | 824         | 838          | rVB3     | 11966          | 34767         | 1.22%           | 0.267%        |
| 13        | 6.763       | 921           | 931         | 951          | rBV      | 356612         | 853580        | 30.04%          | 6.555%        |
| 14        | 7.208       | 997           | 1004        | 1022         | rBV      | 102664         | 240867        | 8.48%           | 1.850%        |
| 15        | 7.580       | 1058          | 1065        | 1075         | rBV      | 55542          | 113473        | 3.99%           | 0.871%        |
| 16        | 8.653       | 1233          | 1241        | 1248         | rBV      | 728433         | 1177975       | 41.46%          | 9.046%        |
| 17        | 10.055      | 1465          | 1471        | 1482         | rBV      | 796392         | 1068803       | 37.61%          | 8.208%        |
| 18        | 10.305      | 1505          | 1512        | 1520         | rVB      | 18113          | 28618         | 1.01%           | 0.220%        |
| 19        | 10.750      | 1581          | 1585        | 1600         | rBV      | 118222         | 181734        | 6.40%           | 1.396%        |
| 20        | 11.079      | 1634          | 1639        | 1645         | rBV      | 656238         | 832589        | 29.30%          | 6.394%        |
| 21        | 11.134      | 1645          | 1648        | 1654         | rVB2     | 25058          | 34188         | 1.20%           | 0.263%        |
| 22        | 11.573      | 1715          | 1720        | 1723         | rBV      | 54307          | 75264         | 2.65%           | 0.578%        |
| 23        | 11.604      | 1723          | 1725        | 1734         | rVV      | 53487          | 71669         | 2.52%           | 0.550%        |
| 24        | 11.866      | 1765          | 1768        | 1778         | rVV2     | 41111          | 66888         | 2.35%           | 0.514%        |
| 25        | 12.024      | 1789          | 1794        | 1801         | rVB      | 875741         | 1115691       | 39.26%          | 8.568%        |
| 26        | 12.219      | 1820          | 1826        | 1837         | rBV      | 1115668        | 1478363       | 52.03%          | 11.353%       |
| 27        | 12.305      | 1838          | 1840        | 1852         | rVB8     | 18707          | 43909         | 1.55%           | 0.337%        |
| 28        | 13.749      | 2072          | 2077        | 2085         | rBV3     | 59516          | 103354        | 3.64%           | 0.794%        |

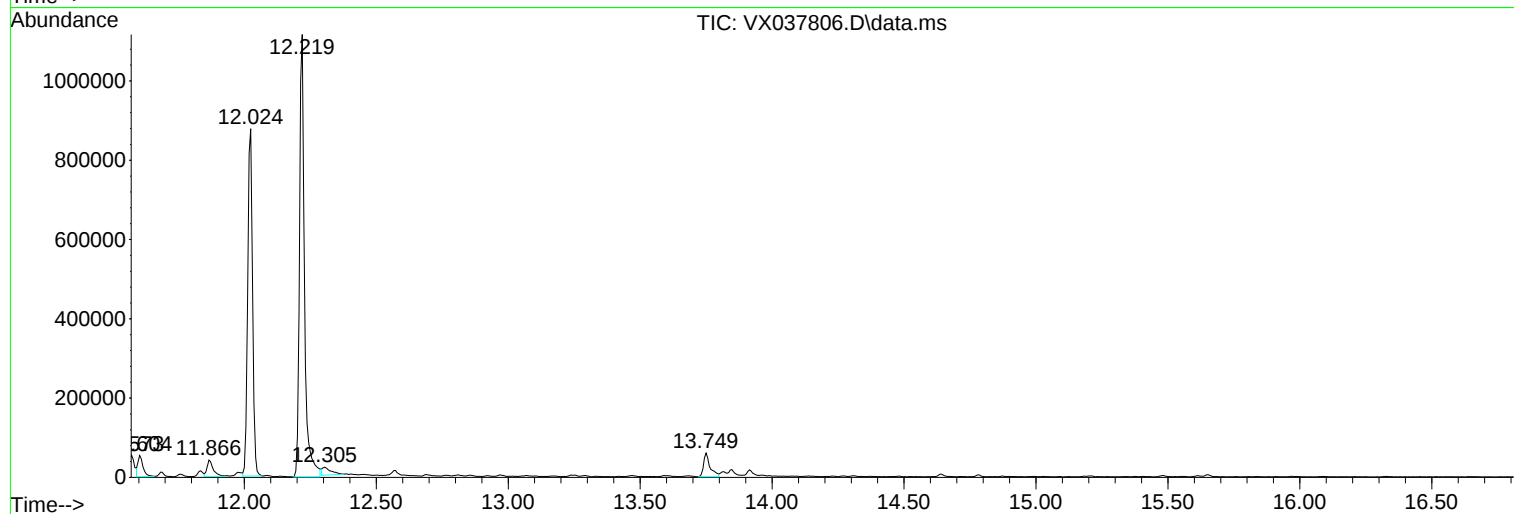
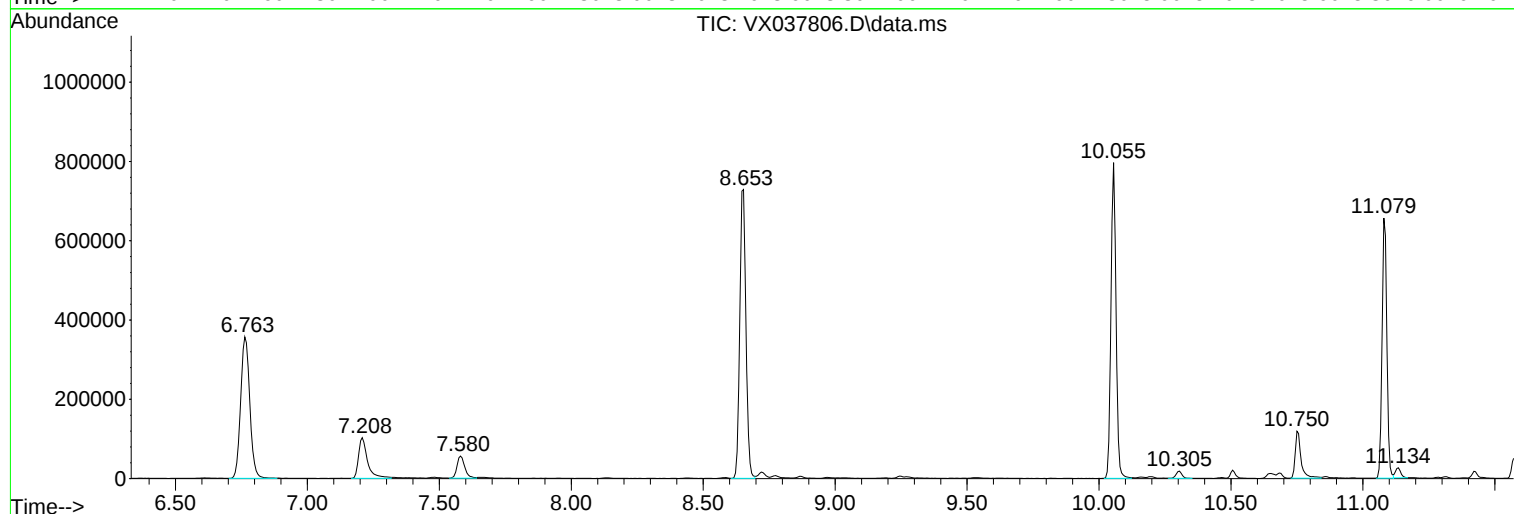
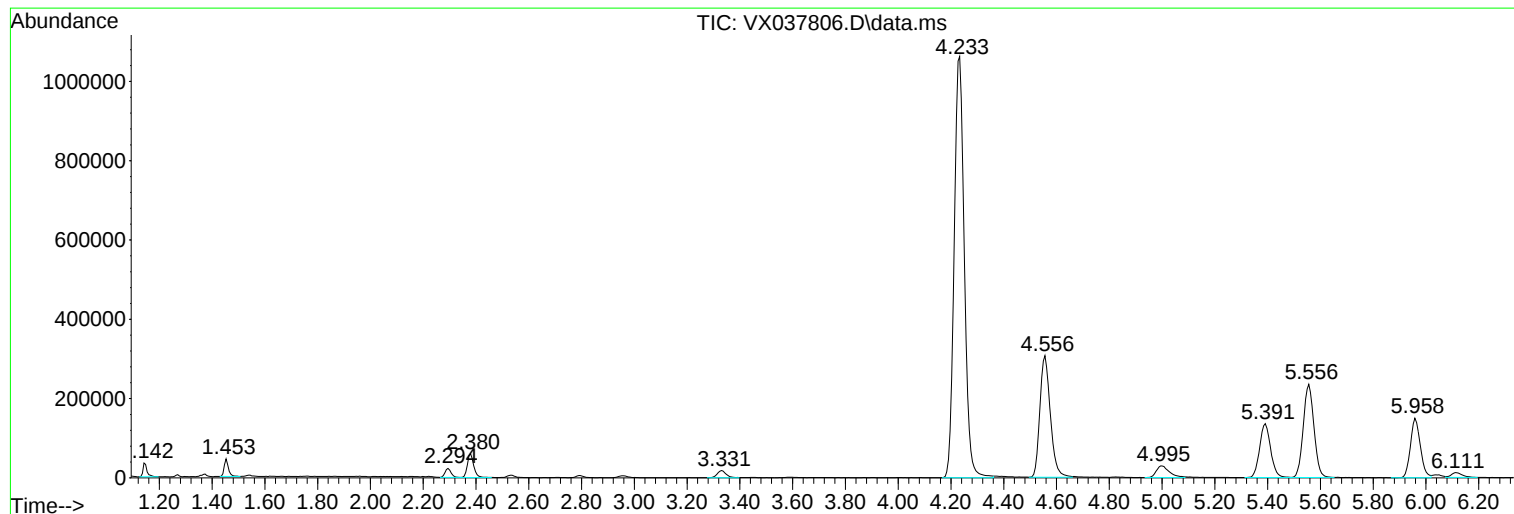
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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

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



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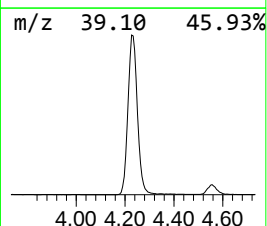
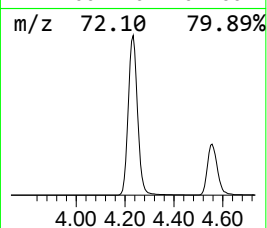
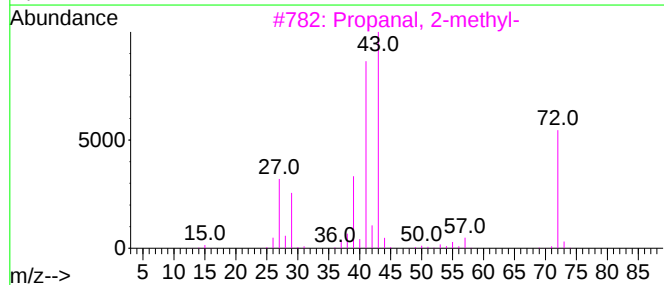
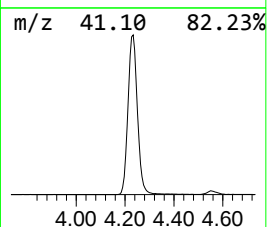
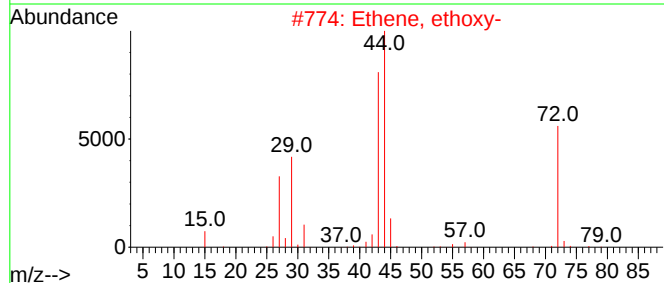
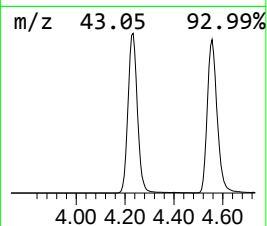
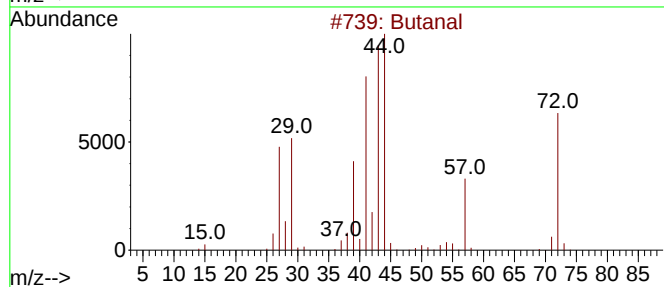
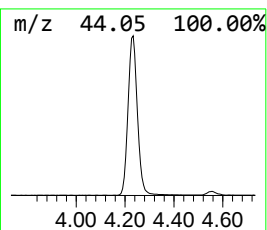
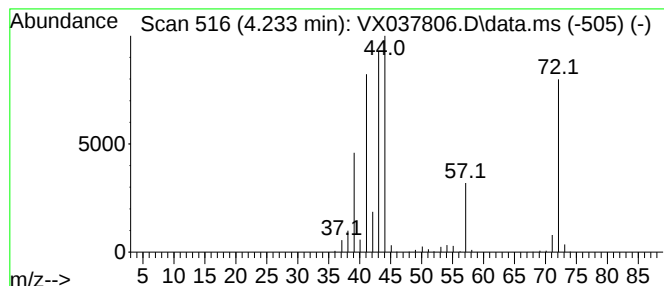
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

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

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Peak Number 1 Butanal Concentration Rank 1

| R.T.  | EstConc     | Area    | Relative to ISTD   | R.T.  |
|-------|-------------|---------|--------------------|-------|
| 4.233 | 214.66 ug/l | 2841440 | Pentafluorobenzene | 5.556 |

| 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 | 58   |
| 3    |    |   | Propanal, 2-methyl-    | 72 | C4H8O   | 000078-84-2 | 46   |
| 4    |    |   | 2-Propanone, hydrazone | 72 | C3H8N2  | 005281-20-9 | 43   |
| 5    |    |   | 1-Propene, 3-methoxy-  | 72 | C4H8O   | 000627-40-7 | 38   |



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ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
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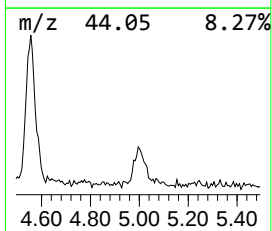
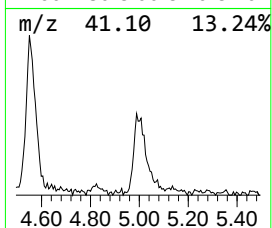
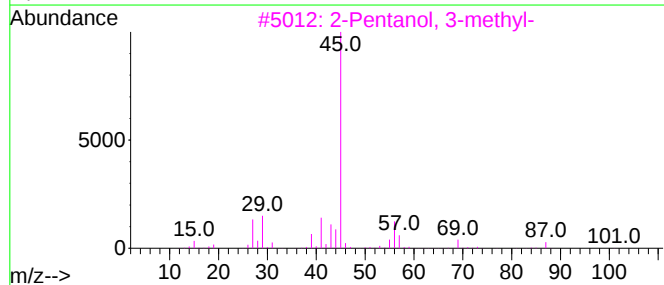
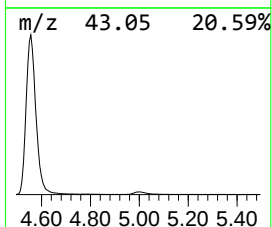
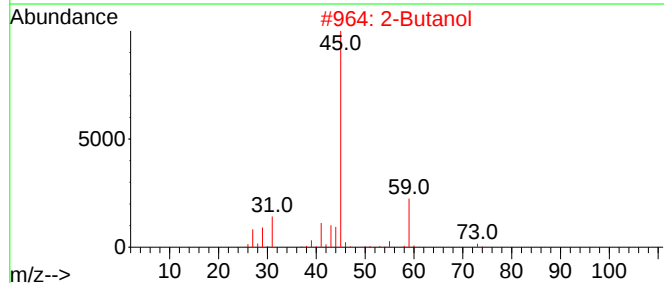
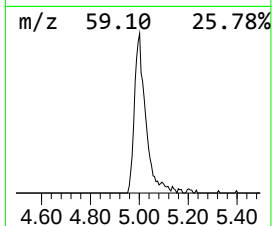
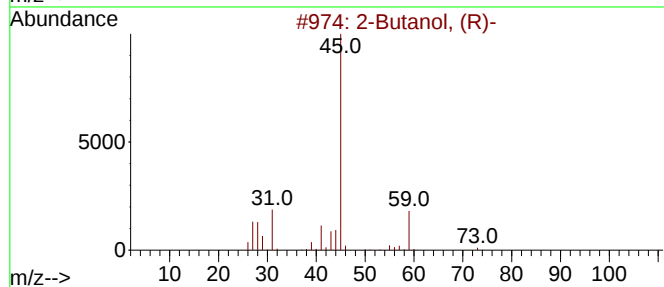
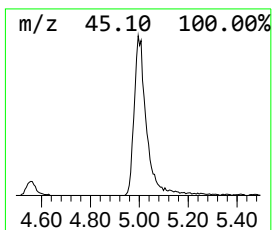
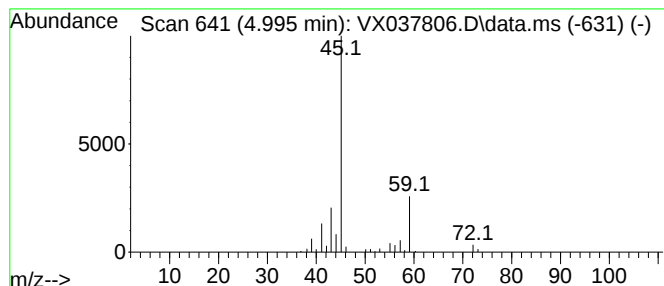
Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

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

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Peak Number 2 2-Butanol, (R)- Concentration Rank 5

| R.T.  | EstConc   | Area   | Relative to ISTD   | R.T.  |
|-------|-----------|--------|--------------------|-------|
| 4.995 | 7.69 ug/l | 101783 | Pentafluorobenzene | 5.556 |

| Hit# | of                     | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|------------------------|---|--------------|-----|---------|-------------|------|
| 1    | 2-Butanol, (R)-        |   |              | 74  | C4H10O  | 014898-79-4 | 83   |
| 2    | 2-Butanol              |   |              | 74  | C4H10O  | 000078-92-2 | 78   |
| 3    | 2-Pentanol, 3-methyl-  |   |              | 102 | C6H14O  | 000565-60-6 | 59   |
| 4    | Isopropyl Alcohol      |   |              | 60  | C3H8O   | 000067-63-0 | 45   |
| 5    | 1-Pentanol, 5-methoxy- |   |              | 118 | C6H14O2 | 004799-62-6 | 38   |



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Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

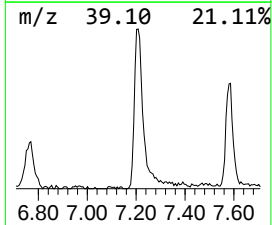
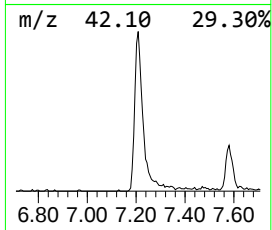
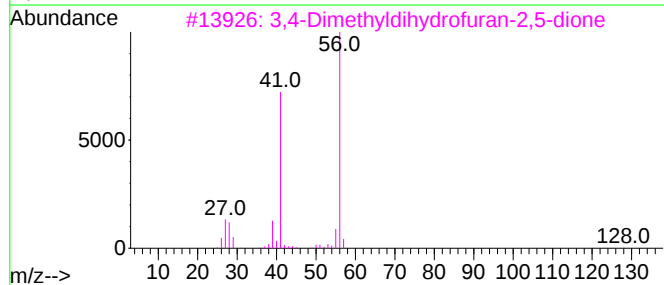
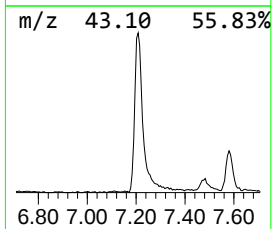
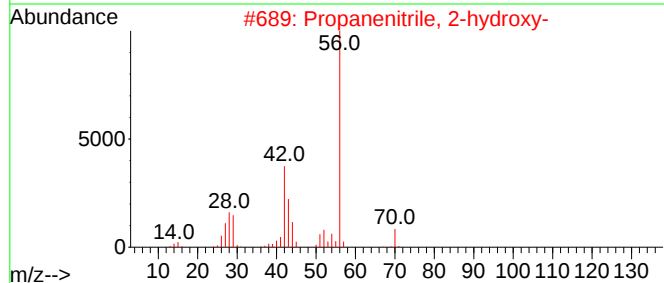
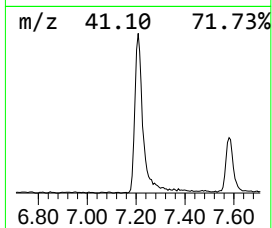
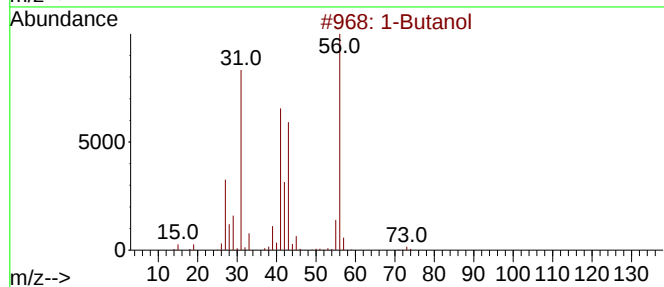
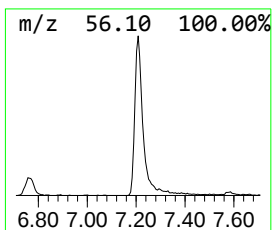
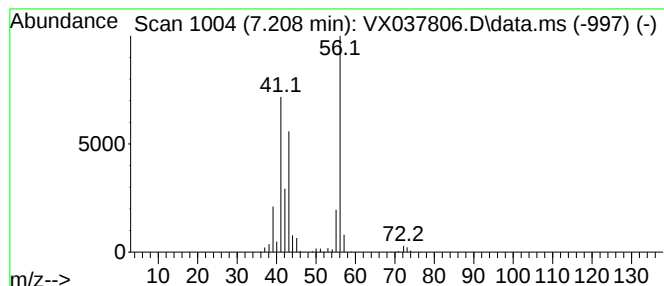
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 1-Butanol Concentration Rank 3

| R.T.  | EstConc    | Area   | Relative to ISTD    | R.T.  |
|-------|------------|--------|---------------------|-------|
| 7.208 | 14.11 ug/l | 240867 | 1,4-Difluorobenzene | 6.763 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 1-Butanol                          | 74  | C4H10O  | 000071-36-3 | 86   |
| 2    |    |   | Propanenitrile, 2-hydroxy-         | 71  | C3H5NO  | 000078-97-7 | 56   |
| 3    |    |   | 3,4-Dimethyldihydrofuran-2,5-dione | 128 | C6H8O3  | 007475-92-5 | 42   |
| 4    |    |   | Propane, 2-cyclopropyl-            | 84  | C6H12   | 003638-35-5 | 38   |
| 5    |    |   | Butane, 1-chloro-                  | 92  | C4H9Cl  | 000109-69-3 | 9    |



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MSVOA\_X  
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Quant Title : SW846 8260

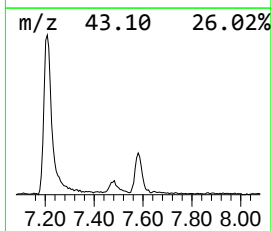
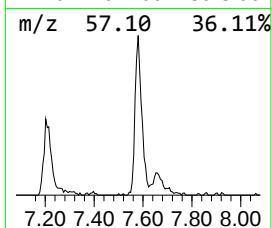
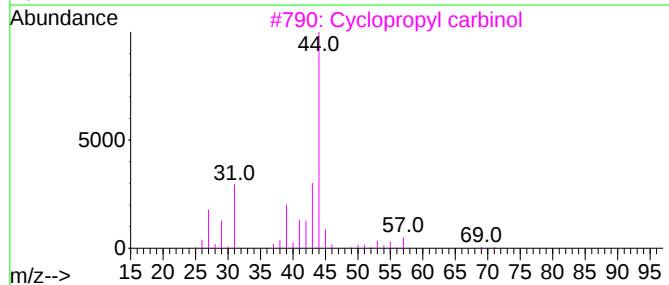
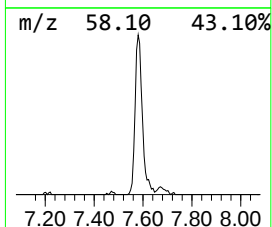
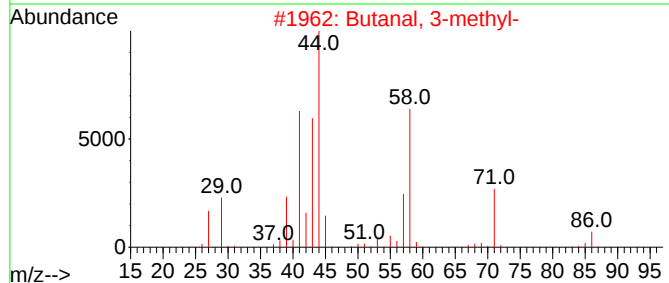
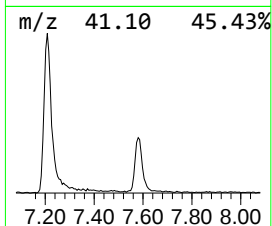
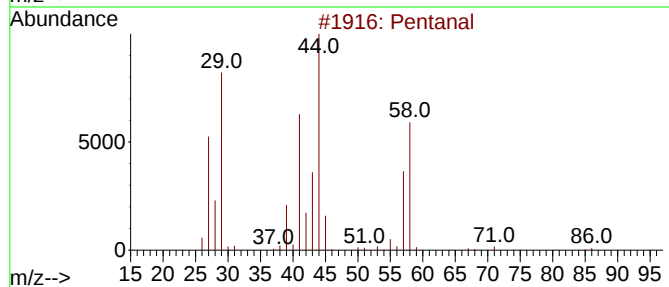
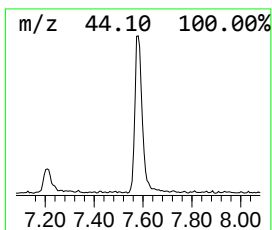
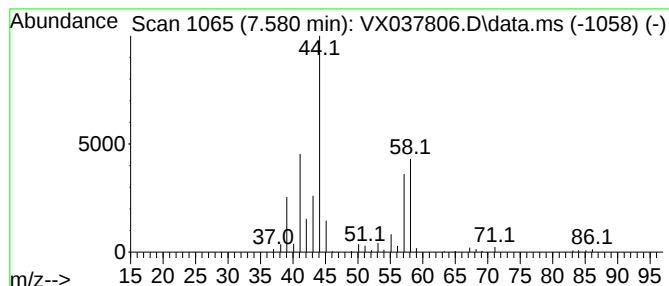
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Pentanal Concentration Rank 6

| R.T.  | EstConc   | Area   | Relative to ISTD    | R.T.  |
|-------|-----------|--------|---------------------|-------|
| 7.580 | 6.65 ug/l | 113473 | 1,4-Difluorobenzene | 6.763 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#         | Qual |
|------|----|---|----------------------|-----|---------|--------------|------|
| 1    |    |   | Pentanal             | 86  | C5H10O  | 000110-62-3  | 87   |
| 2    |    |   | Butanal, 3-methyl-   | 86  | C5H10O  | 000590-86-3  | 74   |
| 3    |    |   | Cyclopropyl carbinol | 72  | C4H8O   | 002516-33-8  | 38   |
| 4    |    |   | Succindialdehyde     | 86  | C4H6O2  | 000638-37-9  | 9    |
| 5    |    |   | 2-Formylhistamine    | 139 | C6H9N3O | 1000132-95-8 | 9    |



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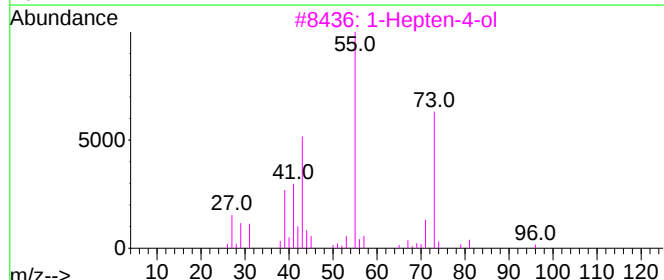
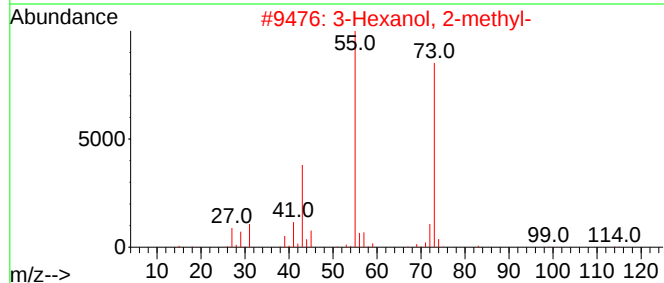
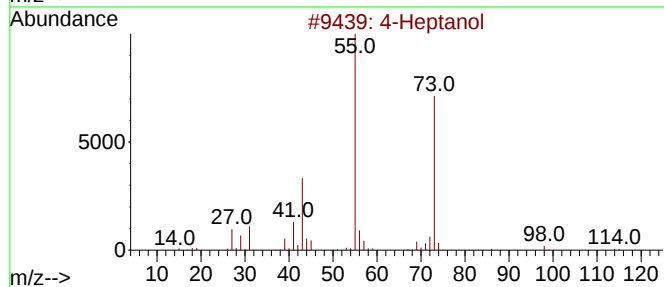
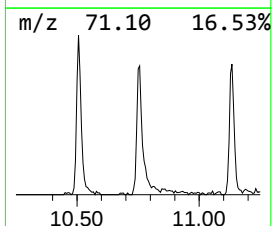
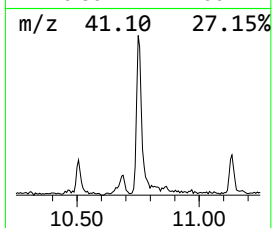
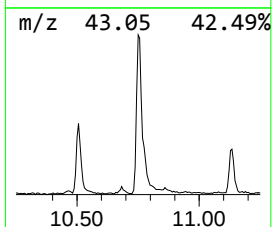
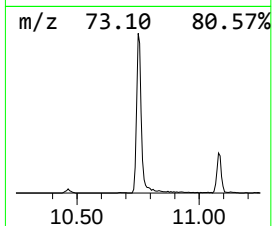
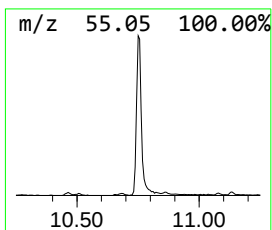
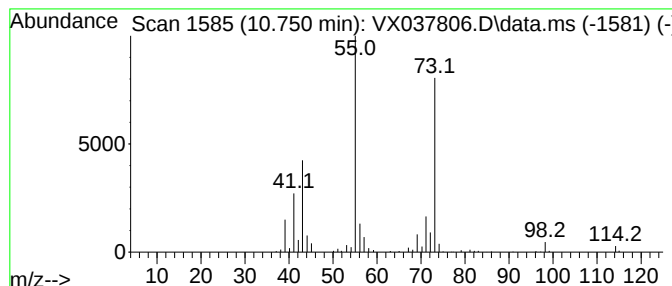
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Quant Title : SW846 8260

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

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Peak Number 5 4-Heptanol Concentration Rank 4

| R.T.   | EstConc   | Area   | Relative to ISTD | R.T.   |
|--------|-----------|--------|------------------|--------|
| 10.750 | 8.50 ug/l | 181734 | Chlorobenzene-d5 | 10.055 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | 4-Heptanol           | 116 | C7H16O  | 000589-55-9 | 78   |
| 2    |    |   | 3-Hexanol, 2-methyl- | 116 | C7H16O  | 000617-29-8 | 50   |
| 3    |    |   | 1-Hepten-4-ol        | 114 | C7H14O  | 003521-91-3 | 50   |
| 4    |    |   | Isobutylamine        | 73  | C4H11N  | 000078-81-9 | 37   |
| 5    |    |   | 5-Hydroxy-4-octanone | 144 | C8H16O2 | 000496-77-5 | 33   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX091923\  
Data File : VX037806.D  
Acq On : 19 Sep 2023 15:16  
Operator : JC/MD  
Sample : 04479-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

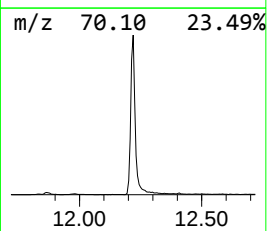
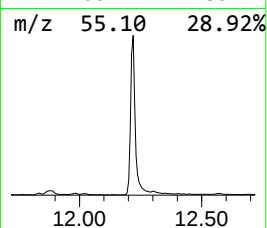
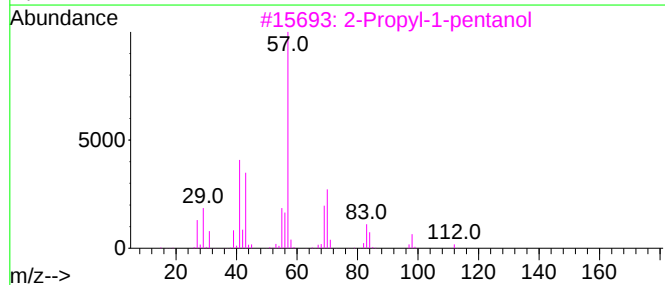
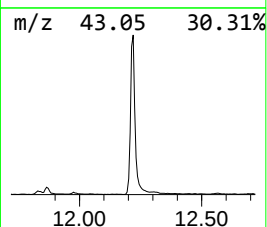
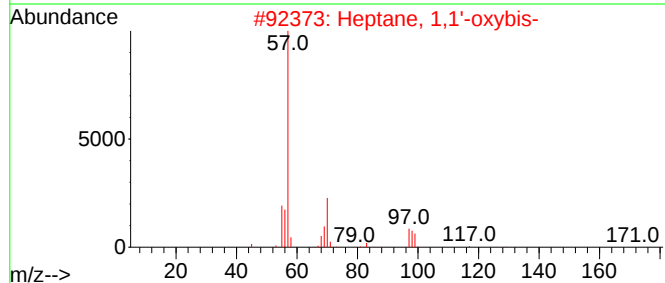
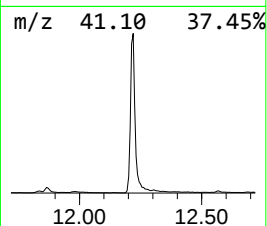
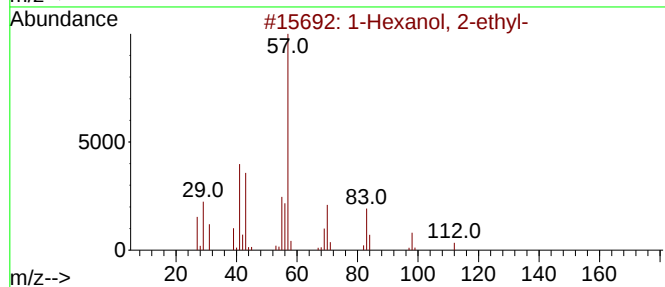
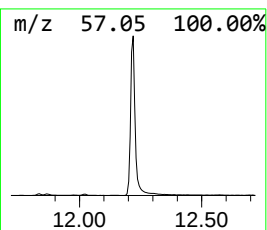
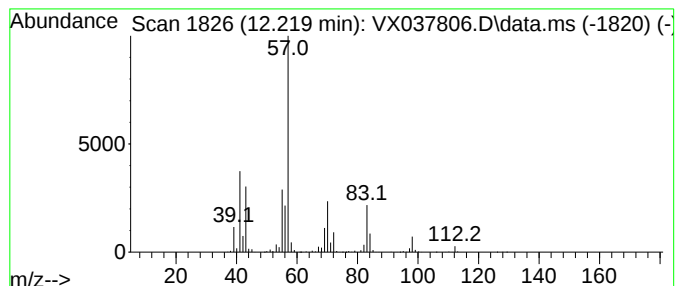
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 2

| R.T.   | EstConc    | Area    | Relative to ISTD       | R.T.   |
|--------|------------|---------|------------------------|--------|
| 12.219 | 66.25 ug/l | 1478360 | 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    |    |   | Heptane, 1,1'-oxybis-               | 214 | C14H30O  | 000629-64-1  | 50   |
| 3    |    |   | 2-Propyl-1-pentanol                 | 130 | C8H18O   | 058175-57-8  | 47   |
| 4    |    |   | Heptyl isobutyl carbonate           | 216 | C12H24O3 | 959068-08-7  | 43   |
| 5    |    |   | Carbonic acid, heptyl prop-1-en-... | 200 | C11H20O3 | 1000382-54-1 | 43   |



Data Path : Z:\voasrv\HPCHEM1\MSVOA\_X\Data\VX091923\  
Data File : VX037806.D  
Acq On : 19 Sep 2023 15:16  
Operator : JC/MD  
Sample : 04479-01  
Misc : 5.0mL/MSVOA\_X/WATER  
ALS Vial : 16 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
1026

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_X\Method\82X091523W.M  
Quant Title : SW846 8260

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butanal            | 4.233  | 214.7   | ug/l  | 2841440  | 1                     | 5.556  | 661838  | 50.0 |
| 2-Butanol, (R)-    | 4.995  | 7.7     | ug/l  | 101783   | 1                     | 5.556  | 661838  | 50.0 |
| 1-Butanol          | 7.208  | 14.1    | ug/l  | 240867   | 2                     | 6.763  | 853580  | 50.0 |
| Pentanal           | 7.580  | 6.7     | ug/l  | 113473   | 2                     | 6.763  | 853580  | 50.0 |
| 4-Heptanol         | 10.750 | 8.5     | ug/l  | 181734   | 3                     | 10.055 | 1068800 | 50.0 |
| 1-Hexanol, 2-et... | 12.219 | 66.3    | ug/l  | 1478360  | 4                     | 12.024 | 1115690 | 50.0 |