

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
 Data File : VN053301.D  
 Acq On : 7 Jan 2019 13:41  
 Operator : MD\SY  
 Sample : K1053-04  
 Misc : 5.00mL/MSVOA N/WATER  
 ALS Vial : 10 Sample Multiplier: 28

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 COMP-2-DRUM

## 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\82N010519W.M  
 Title : SW846 8260

Signal : TIC

| 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         | 2.310       | 153           | 167         | 212          | rBV2     | 24395395       | 40219780      | 100.00%         | 52.058%       |
| 2         | 3.265       | 446           | 464         | 511          | rBV      | 1839362        | 4315298       | 10.73%          | 5.585%        |
| 3         | 6.542       | 1460          | 1483        | 1509         | rBV      | 1053039        | 3142560       | 7.81%           | 4.068%        |
| 4         | 6.834       | 1551          | 1574        | 1595         | rBV      | 698759         | 1993988       | 4.96%           | 2.581%        |
| 5         | 7.593       | 1790          | 1810        | 1820         | rBV      | 576994         | 1422947       | 3.54%           | 1.842%        |
| 6         | 7.667       | 1821          | 1833        | 1860         | rVB      | 1150604        | 2694574       | 6.70%           | 3.488%        |
| 7         | 8.027       | 1924          | 1945        | 1974         | rBV2     | 688568         | 1709661       | 4.25%           | 2.213%        |
| 8         | 8.587       | 2103          | 2119        | 2136         | rVB      | 1658578        | 3433771       | 8.54%           | 4.444%        |
| 9         | 10.091      | 2570          | 2587        | 2600         | rBV      | 2731934        | 4991058       | 12.41%          | 6.460%        |
| 10        | 10.853      | 2802          | 2824        | 2848         | rBV2     | 236771         | 507699        | 1.26%           | 0.657%        |
| 11        | 11.406      | 2981          | 2996        | 3019         | rVB      | 2451275        | 4242856       | 10.55%          | 5.492%        |
| 12        | 12.400      | 3291          | 3305        | 3320         | rBV      | 2080809        | 3449180       | 8.58%           | 4.464%        |
| 13        | 12.914      | 3452          | 3465        | 3479         | rVB      | 362471         | 564782        | 1.40%           | 0.731%        |
| 14        | 13.342      | 3585          | 3598        | 3616         | rVB      | 2374306        | 3938431       | 9.79%           | 5.098%        |
| 15        | 13.451      | 3618          | 3632        | 3648         | rBV2     | 363759         | 633401        | 1.57%           | 0.820%        |

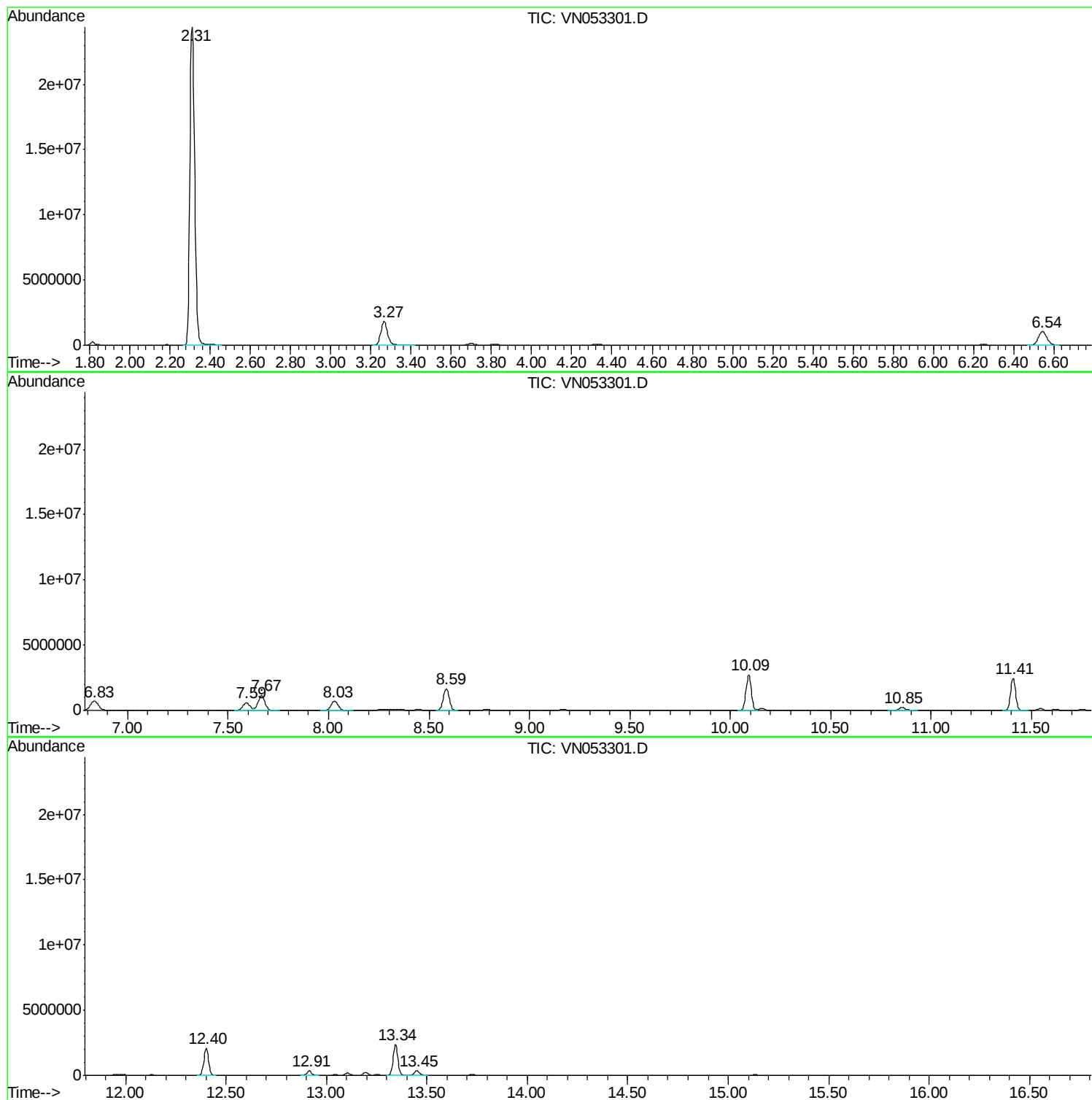
Sum of corrected areas: 77259986

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

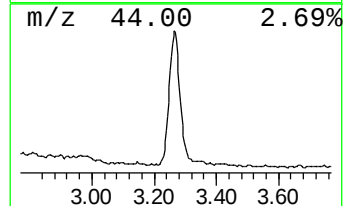
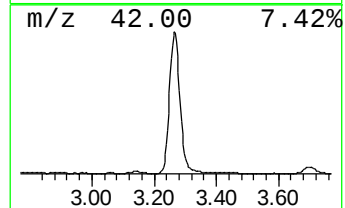
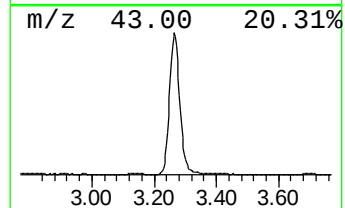
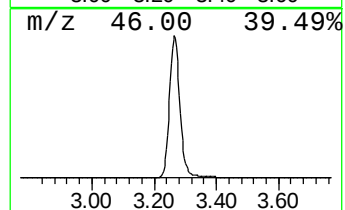
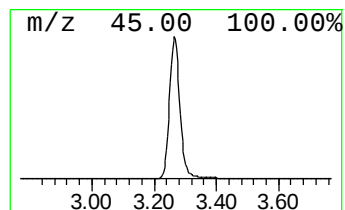
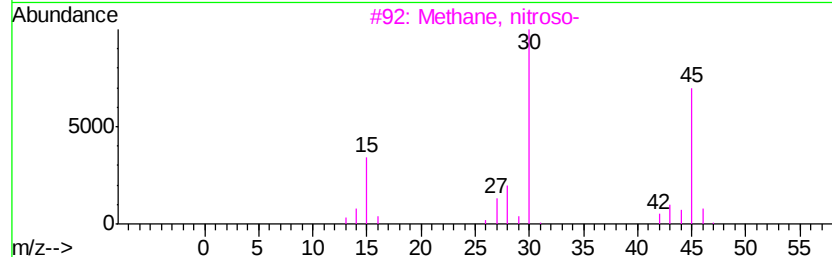
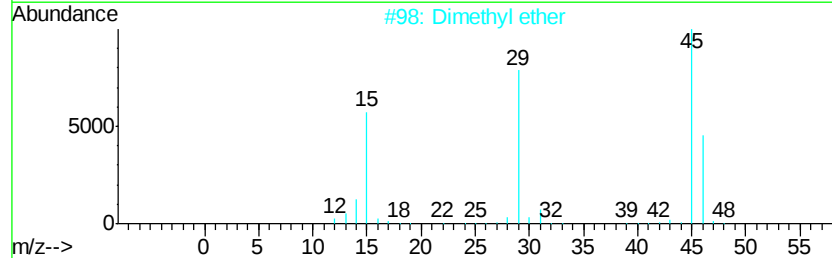
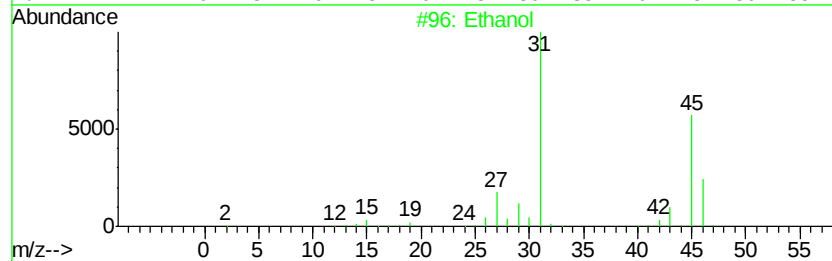
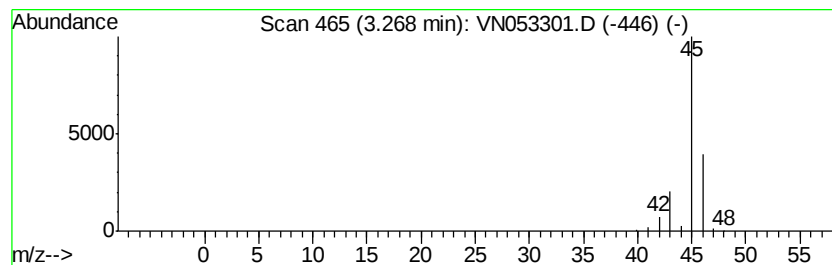
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 Ethanol Concentration Rank 2

| R.T. | EstConc    | Area    | Relative to ISTD   | R.T. |
|------|------------|---------|--------------------|------|
| 3.27 | 80.07 ug/l | 4315300 | Pentafluorobenzene | 7.67 |

| Hit# | of | Tentative ID      | MW | MolForm | CAS#        | Qual |
|------|----|-------------------|----|---------|-------------|------|
| 1    | 5  | 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    |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

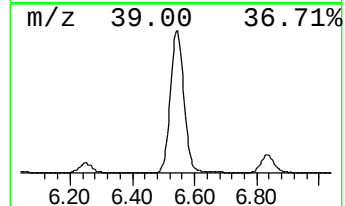
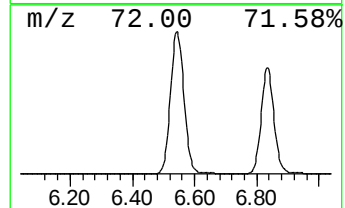
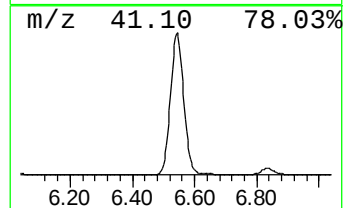
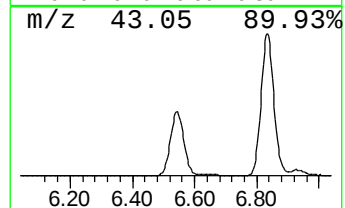
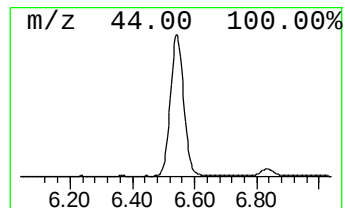
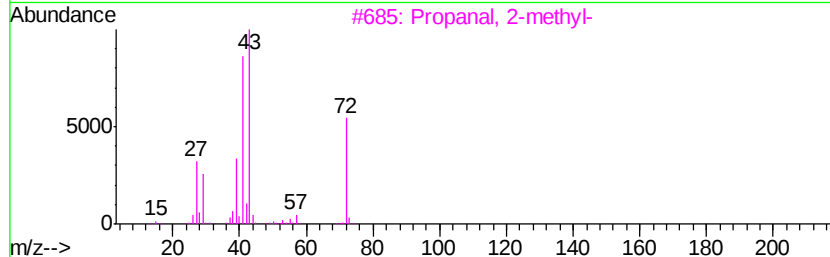
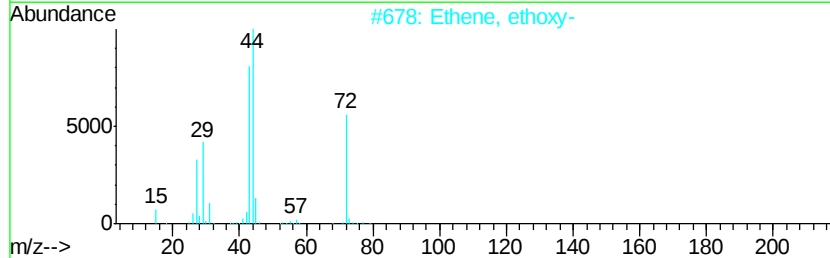
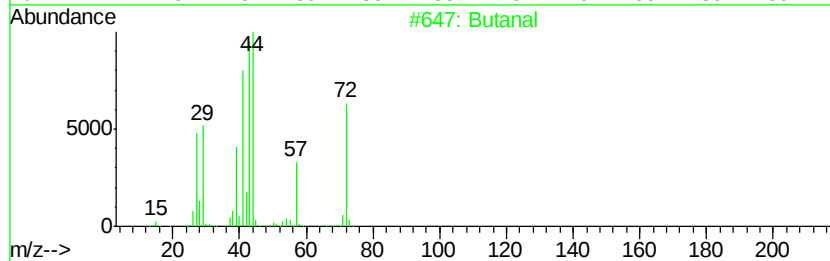
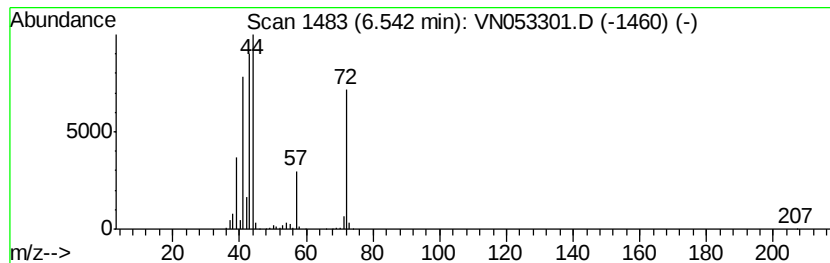
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 Butanal Concentration Rank 3

| R.T. | EstConc    | Area    | Relative to ISTD   | R.T. |
|------|------------|---------|--------------------|------|
| 6.54 | 58.31 ug/l | 3142560 | Pentafluorobenzene | 7.67 |

| Hit# | of | Tentative ID          | MW | MolForm | CAS#        | Qual |
|------|----|-----------------------|----|---------|-------------|------|
| 1    | 5  | Butanal               | 72 | C4H8O   | 000123-72-8 | 94   |
| 2    |    | Ethene, ethoxy-       | 72 | C4H8O   | 000109-92-2 | 64   |
| 3    |    | Propanal, 2-methyl-   | 72 | C4H8O   | 000078-84-2 | 46   |
| 4    |    | Isobutylene epoxide   | 72 | C4H8O   | 000558-30-5 | 27   |
| 5    |    | 1-Propene, 3-methoxy- | 72 | C4H8O   | 000627-40-7 | 27   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

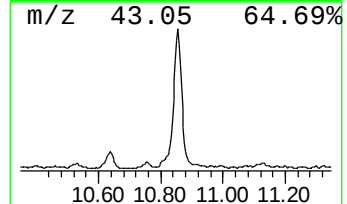
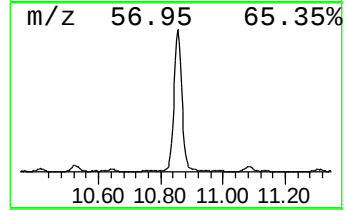
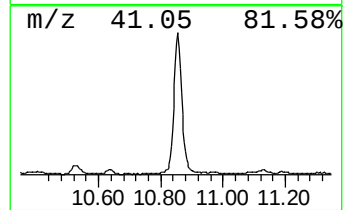
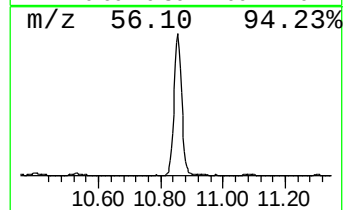
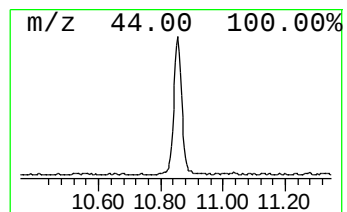
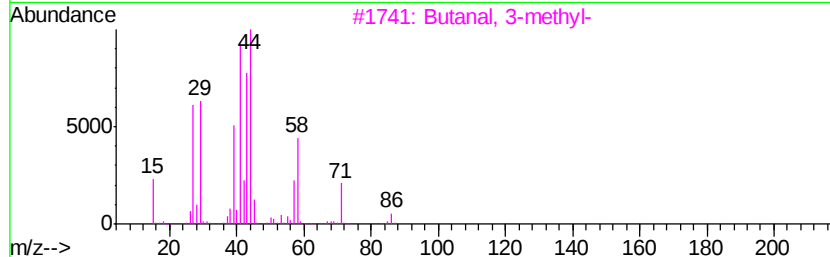
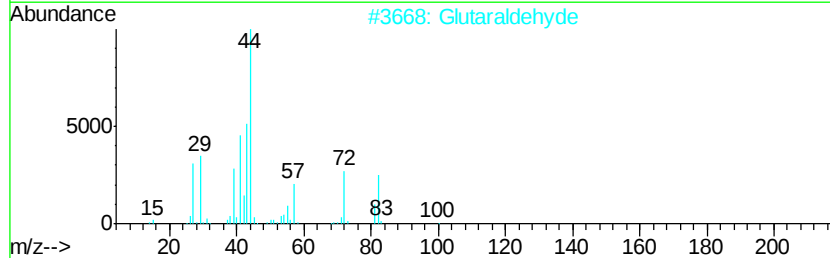
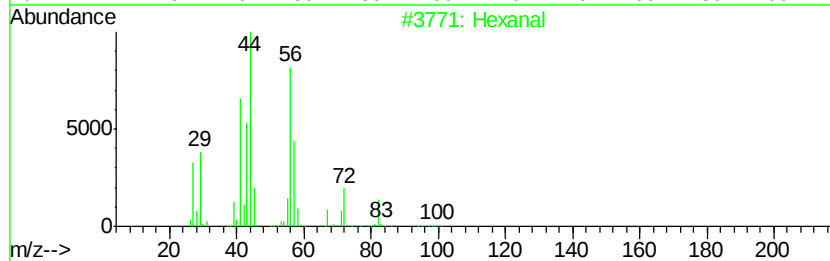
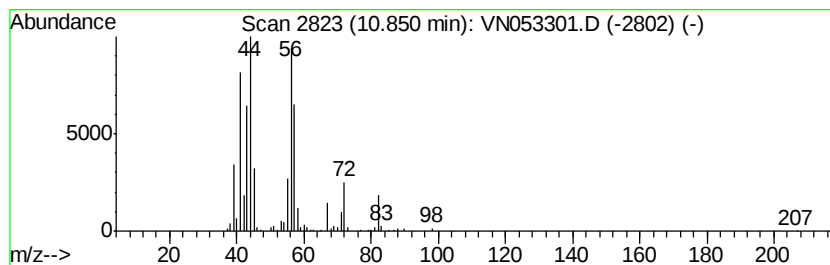
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Hexanal Concentration Rank 6

| R.T.  | EstConc   | Area   | Relative to ISTD | R.T.  |
|-------|-----------|--------|------------------|-------|
| 10.85 | 5.98 ug/l | 507699 | Chlorobenzene-d5 | 11.41 |

| Hit# of | 5                  | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|--------------------|--------------|-----|---------|-------------|------|
| 1       | Hexanal            |              | 100 | C6H12O  | 000066-25-1 | 90   |
| 2       | Glutaraldehyde     |              | 100 | C5H8O2  | 000111-30-8 | 32   |
| 3       | Butanal, 3-methyl- |              | 86  | C5H10O  | 000590-86-3 | 27   |
| 4       | Butanal            |              | 72  | C4H8O   | 000123-72-8 | 16   |
| 5       | 2-Hexen-1-ol, (E)- |              | 100 | C6H12O  | 000928-95-0 | 14   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

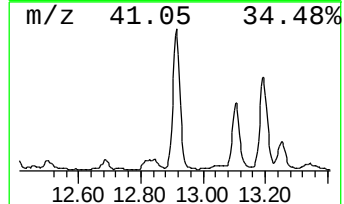
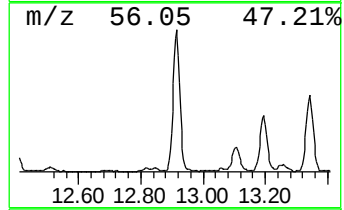
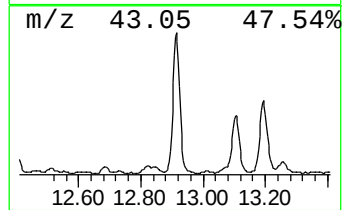
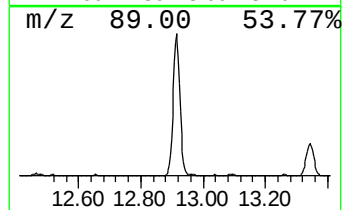
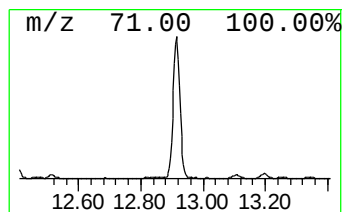
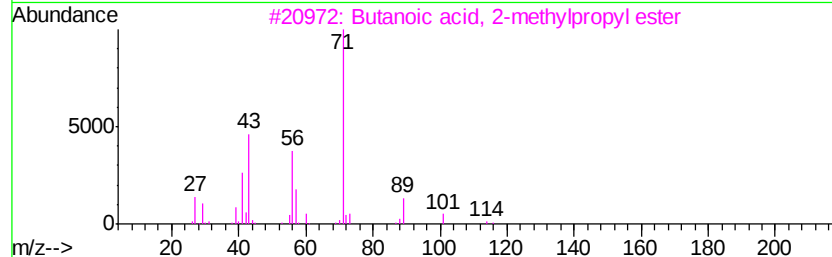
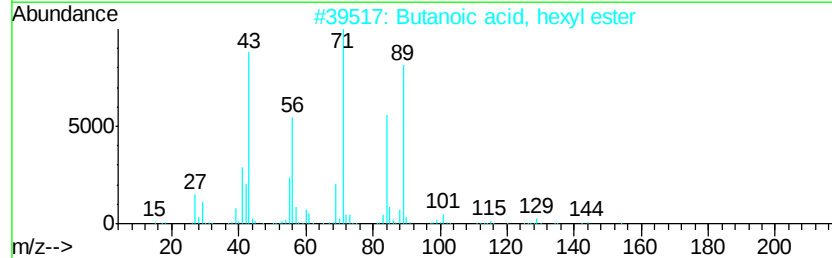
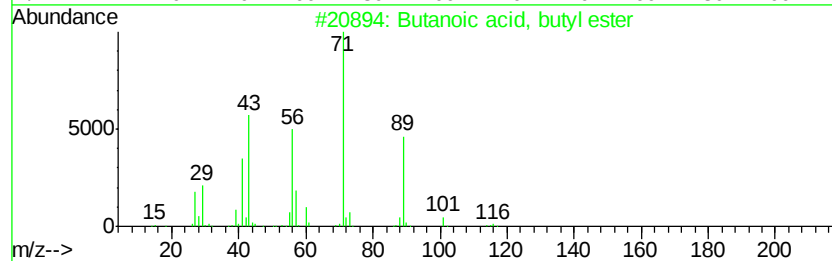
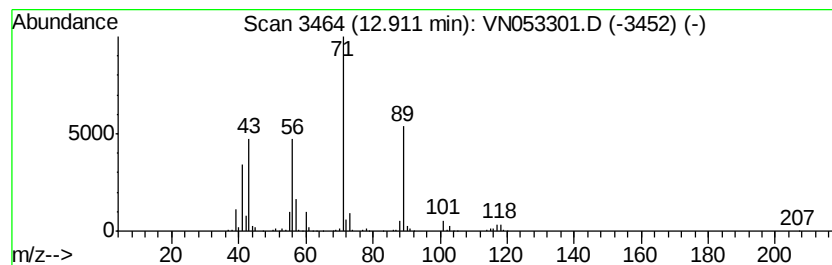
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Butanoic acid, butyl ester Concentration Rank 5

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 12.91 | 7.17 ug/l | 564782 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Butanoic acid, butyl ester          | 144 | C8H16O2  | 000109-21-7 | 90   |
| 2    |    | Butanoic acid, hexyl ester          | 172 | C10H20O2 | 002639-63-6 | 64   |
| 3    |    | Butanoic acid, 2-methylpropyl ester | 144 | C8H16O2  | 000539-90-2 | 64   |
| 4    |    | Butanoic acid, propyl ester         | 130 | C7H14O2  | 000105-66-8 | 45   |
| 5    |    | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2  | 000097-85-8 | 45   |



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampled :  
COMP-2-DRUM

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

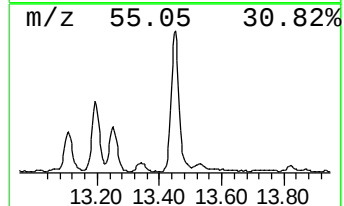
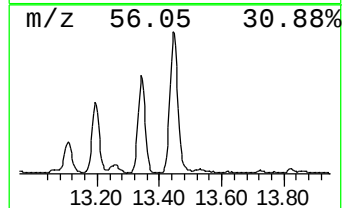
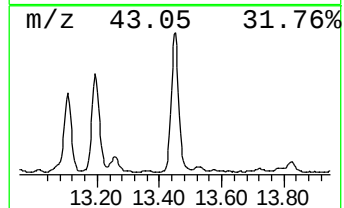
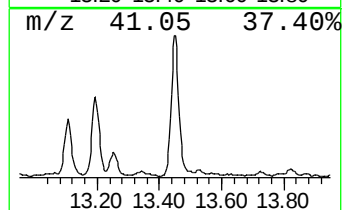
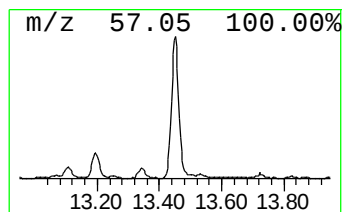
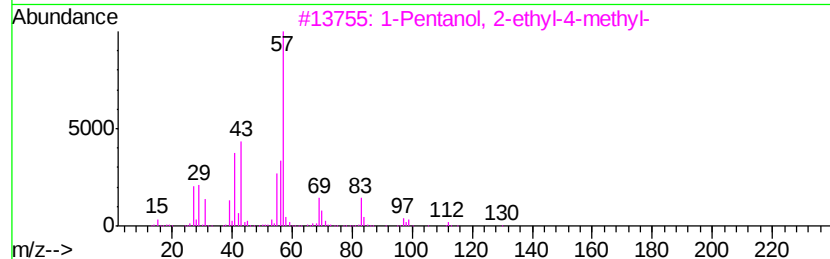
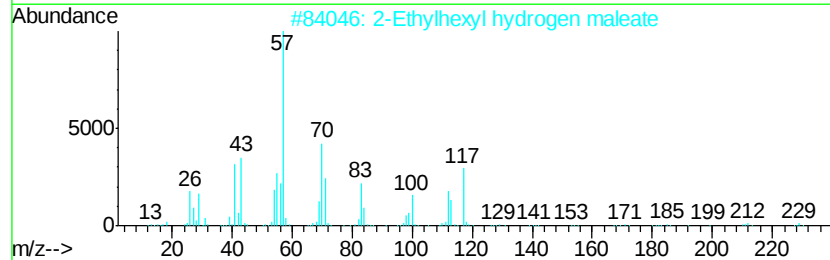
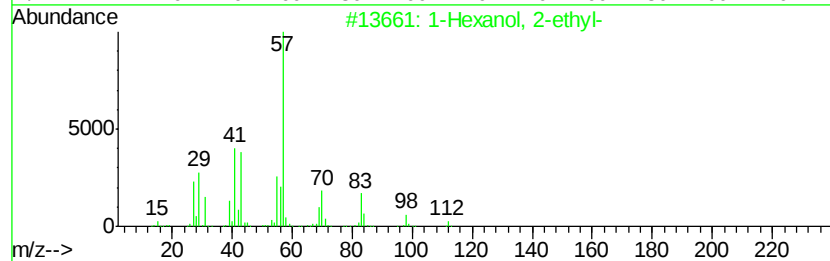
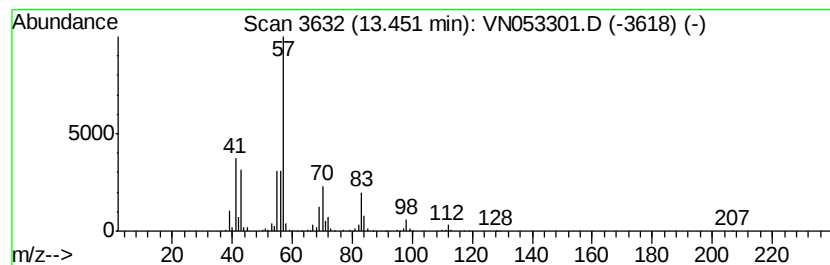
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 1-Hexanol, 2-ethyl- Concentration Rank 4

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 13.45 | 8.04 ug/l | 633401 | 1,4-Dichlorobenzene-d4 | 13.35 |

| Hit# | of | Tentative ID                    | MW  | MolForm  | CAS#         | Qual |
|------|----|---------------------------------|-----|----------|--------------|------|
| 1    | 5  | 1-Hexanol, 2-ethyl-             | 130 | C8H18O   | 000104-76-7  | 72   |
| 2    |    | 2-Ethylhexyl hydrogen maleate   | 228 | C12H20O4 | 002370-71-0  | 59   |
| 3    |    | 1-Pentanol, 2-ethyl-4-methyl-   | 130 | C8H18O   | 000106-67-2  | 59   |
| 4    |    | 2-Ethyl-1-hexanol, methyl ether | 144 | C9H20O   | 1000365-10-2 | 50   |
| 5    |    | 2-Propyl-1-pentanol             | 130 | C8H18O   | 058175-57-8  | 47   |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_N\DATA\VN010719\  
Data File : VN053301.D  
Acq On : 7 Jan 2019 13:41  
Operator : MD\SY  
Sample : K1053-04  
Misc : 5.00mL/MSVOA\_N/WATER  
ALS Vial : 10 Sample Multiplier: 28

Instrument :  
MSVOA\_N  
ClientSampleId :  
COMP-2-DRUM

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_N\METHODS\82N010519W.M  
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | ---Internal Standard--- |       |         |      |
|----------------------|-------|---------|-------|----------|-------------------------|-------|---------|------|
|                      |       |         |       |          | #                       | RT    | Resp    | Conc |
| Ethanol              | 3.27  | 80.1    | ug/l  | 4315300  | 1                       | 7.67  | 2694570 | 50.0 |
| Butanal              | 6.54  | 58.3    | ug/l  | 3142560  | 1                       | 7.67  | 2694570 | 50.0 |
| Hexanal              | 10.85 | 6.0     | ug/l  | 507699   | 3                       | 11.41 | 4242860 | 50.0 |
| Butanoic acid, bu... | 12.91 | 7.2     | ug/l  | 564782   | 4                       | 13.35 | 3938430 | 50.0 |
| 1-Hexanol, 2-ethyl-  | 13.45 | 8.0     | ug/l  | 633401   | 4                       | 13.35 | 3938430 | 50.0 |