

Data Path : Z:\VOASRV\HPCHEM1\MSVOA N\DATA\VN111819\  
 Data File : VN059284.D  
 Acq On : 18 Nov 2019 15:22  
 Operator : JC/SP  
 Sample : IBLK  
 Misc : 5.00mL/MSVOA N/WATER  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_N  
 ClientSampleId :  
 IBLK

Integration Parameters: RTEINT.P

Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA\_N\METHODS\82N110619W.M  
 Title : SW846 8260

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|--------|----------|------------|----------|-----------|-------|-------------|------------|--------------|------------|
| 1      | 1.796    | 3          | 7        | 21        | rVB3  | 19514       | 26703      | 1.17%        | 0.190%     |
| 2      | 2.140    | 105        | 114      | 129       | rVB   | 99467       | 143665     | 6.32%        | 1.021%     |
| 3      | 3.799    | 614        | 630      | 645       | rBV2  | 9962        | 27771      | 1.22%        | 0.197%     |
| 4      | 4.034    | 683        | 703      | 716       | rBV2  | 8419        | 24470      | 1.08%        | 0.174%     |
| 5      | 5.928    | 1268       | 1292     | 1320      | rBV3  | 51434       | 187630     | 8.25%        | 1.334%     |
| 6      | 6.519    | 1453       | 1476     | 1499      | rBV6  | 18153       | 64650      | 2.84%        | 0.460%     |
| 7      | 6.796    | 1543       | 1562     | 1584      | rBV3  | 6945        | 26118      | 1.15%        | 0.186%     |
| 8      | 7.571    | 1784       | 1803     | 1814      | rBV2  | 283539      | 702446     | 30.90%       | 4.994%     |
| 9      | 7.645    | 1814       | 1826     | 1853      | rVB   | 560107      | 1335361    | 58.74%       | 9.494%     |
| 10     | 8.008    | 1919       | 1939     | 1958      | rBV   | 331030      | 789660     | 34.73%       | 5.614%     |
| 11     | 8.567    | 2097       | 2113     | 2136      | rBV   | 783151      | 1649436    | 72.55%       | 11.727%    |
| 12     | 8.773    | 2163       | 2177     | 2203      | rBV3  | 60283       | 141485     | 6.22%        | 1.006%     |
| 13     | 9.400    | 2360       | 2372     | 2387      | rVB3  | 16505       | 32609      | 1.43%        | 0.232%     |
| 14     | 10.082   | 2569       | 2584     | 2598      | rBV   | 1230900     | 2273481    | 100.00%      | 16.164%    |
| 15     | 10.519   | 2713       | 2720     | 2738      | rVB4  | 14926       | 30159      | 1.33%        | 0.214%     |
| 16     | 11.403   | 2981       | 2995     | 3018      | rBV   | 1107833     | 1951096    | 85.82%       | 13.872%    |
| 17     | 11.616   | 3051       | 3061     | 3075      | rVB2  | 49481       | 100116     | 4.40%        | 0.712%     |
| 18     | 11.947   | 3156       | 3164     | 3172      | rBV2  | 22717       | 35722      | 1.57%        | 0.254%     |
| 19     | 11.998   | 3172       | 3180     | 3189      | rVB2  | 21307       | 32963      | 1.45%        | 0.234%     |
| 20     | 12.400   | 3293       | 3305     | 3322      | rBV   | 826035      | 1405923    | 61.84%       | 9.996%     |
| 21     | 12.821   | 3427       | 3436     | 3440      | rBV4  | 14585       | 22852      | 1.01%        | 0.162%     |
| 22     | 12.915   | 3454       | 3465     | 3477      | rBV   | 183663      | 279715     | 12.30%       | 1.989%     |
| 23     | 13.107   | 3518       | 3525     | 3538      | rVB3  | 35542       | 59321      | 2.61%        | 0.422%     |
| 24     | 13.252   | 3561       | 3570     | 3585      | rVB2  | 98931       | 166107     | 7.31%        | 1.181%     |
| 25     | 13.345   | 3586       | 3599     | 3615      | rVB   | 917707      | 1554584    | 68.38%       | 11.053%    |
| 26     | 13.451   | 3620       | 3632     | 3648      | rBV   | 527679      | 888600     | 39.09%       | 6.318%     |
| 27     | 13.725   | 3710       | 3717     | 3729      | rVB   | 36602       | 59189      | 2.60%        | 0.421%     |
| 28     | 14.162   | 3846       | 3853     | 3866      | rBV2  | 30129       | 53091      | 2.34%        | 0.377%     |

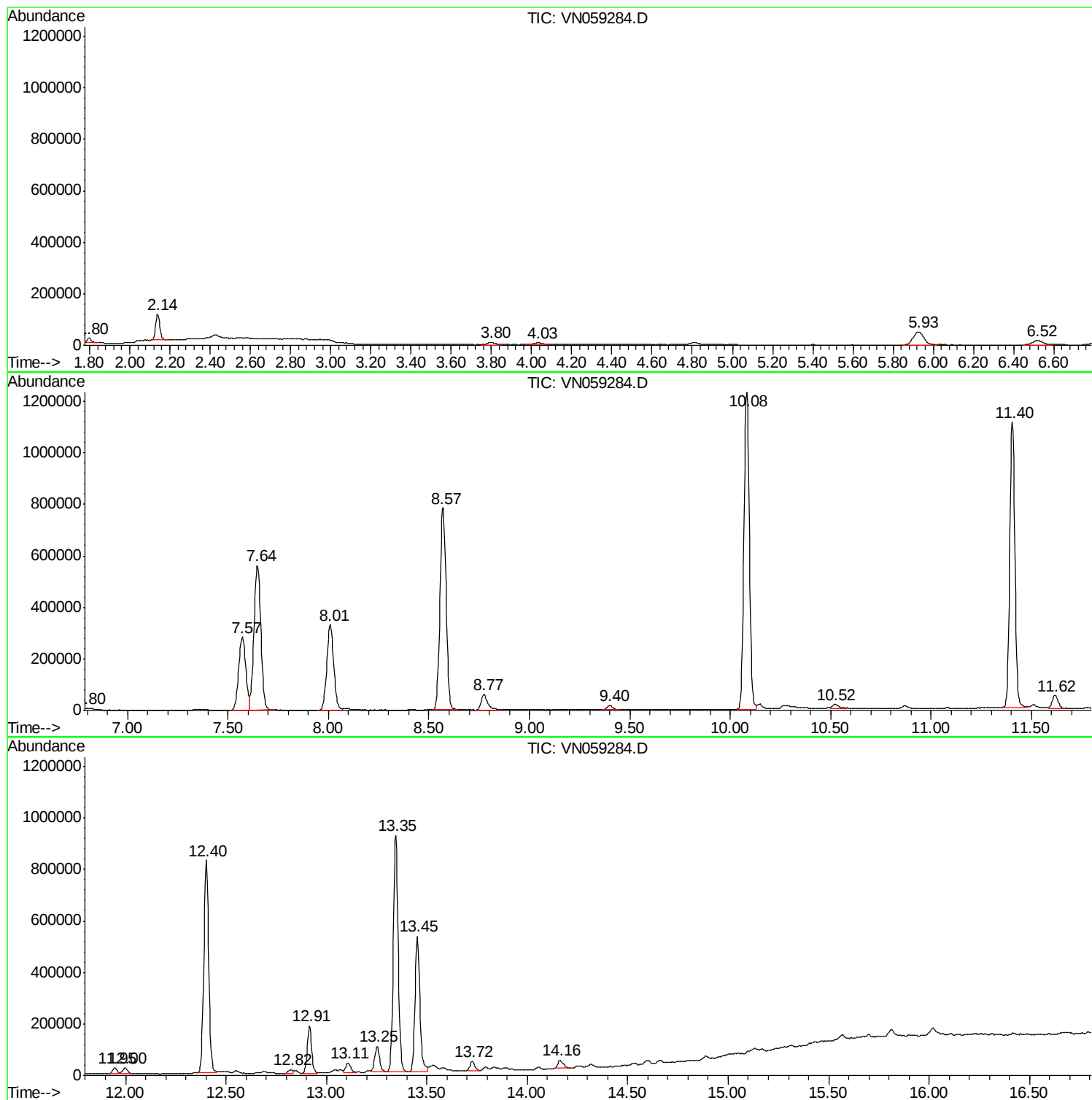
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MSVOA\_N  
ClientSampleId :  
IBLK

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N110619W.M  
Quant Title : SW846 8260

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



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Instrument :  
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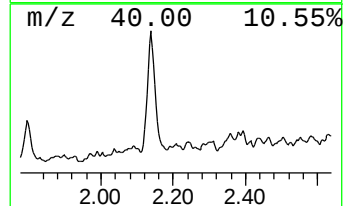
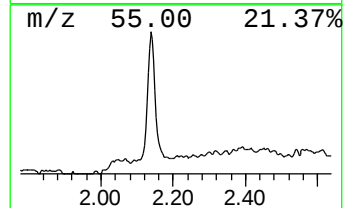
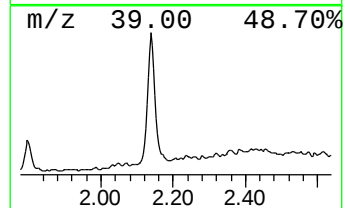
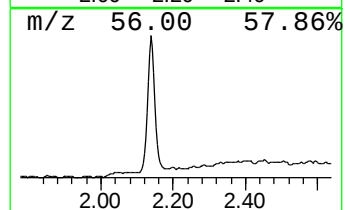
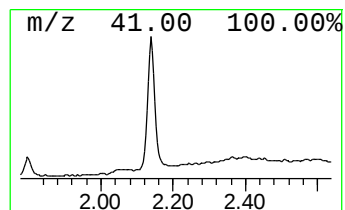
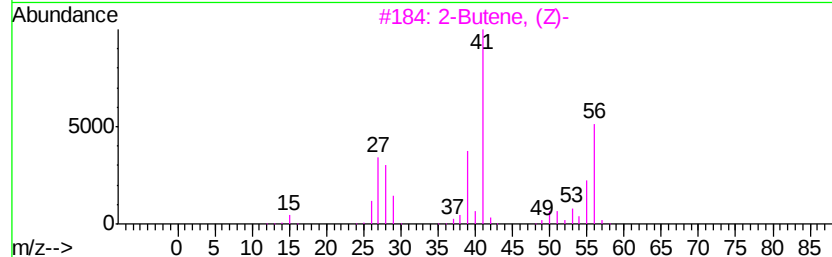
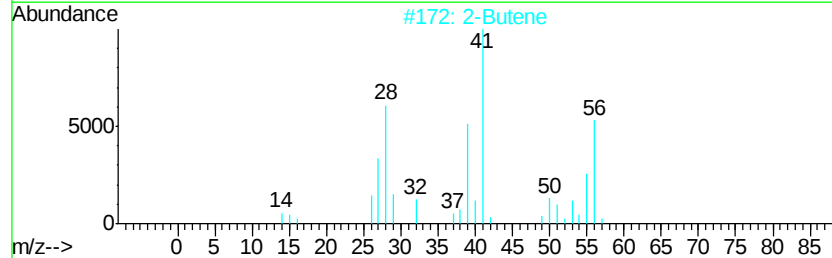
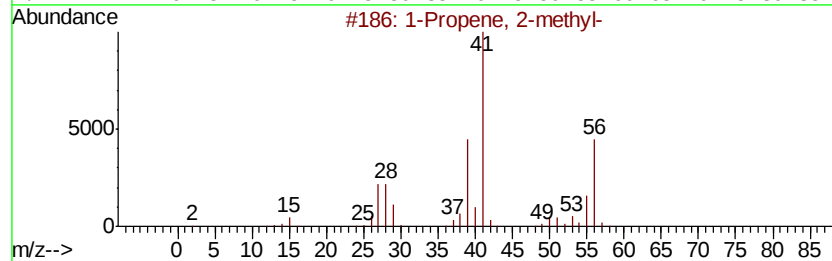
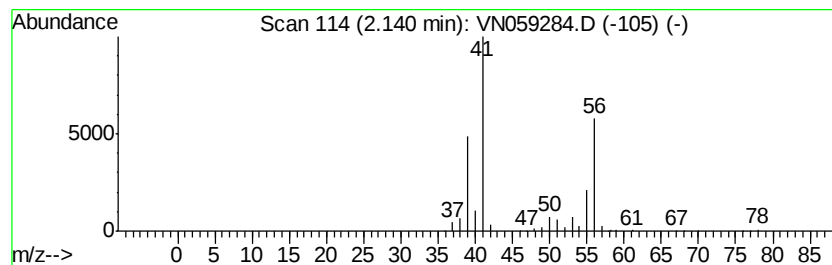
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N110619W.M  
Quant Title : SW846 8260

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

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Peak Number 1 1-Propene, 2-methyl- Concentration Rank 4

| R.T. | EstConc   | Area   | Relative to ISTD   | R.T. |
|------|-----------|--------|--------------------|------|
| 2.14 | 5.38 ug/l | 143665 | Pentafluorobenzene | 7.65 |

| Hit# | of | 5 | Tentative ID         | MW | MolForm | CAS#        | Qual |
|------|----|---|----------------------|----|---------|-------------|------|
| 1    |    |   | 1-Propene, 2-methyl- | 56 | C4H8    | 000115-11-7 | 90   |
| 2    |    |   | 2-Butene             | 56 | C4H8    | 000107-01-7 | 80   |
| 3    |    |   | 2-Butene, (Z)-       | 56 | C4H8    | 000590-18-1 | 80   |
| 4    |    |   | Cyclobutane          | 56 | C4H8    | 000287-23-0 | 49   |
| 5    |    |   | 1-Butene             | 56 | C4H8    | 000106-98-9 | 49   |



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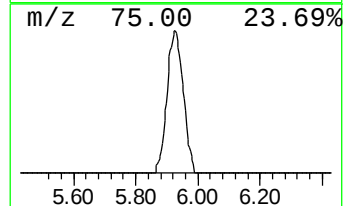
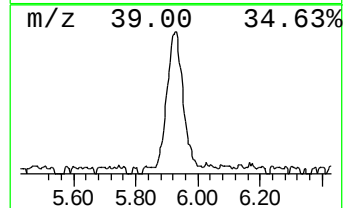
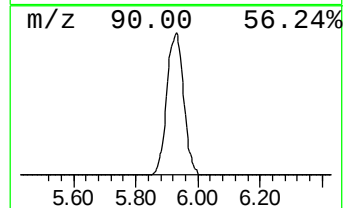
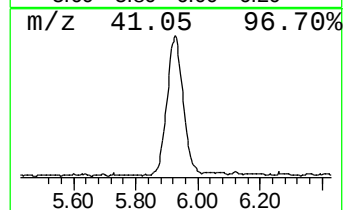
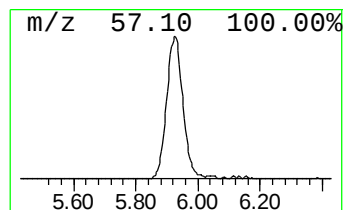
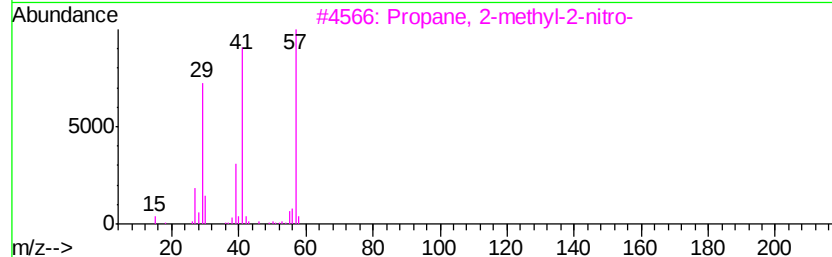
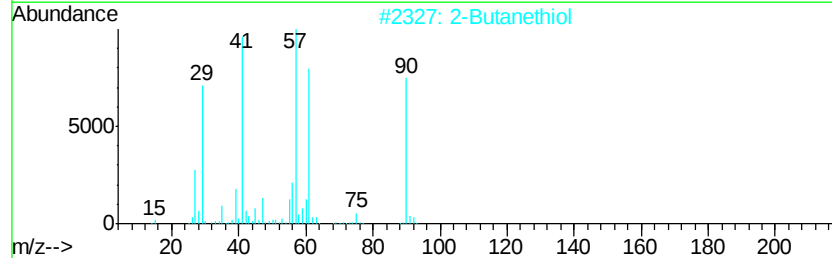
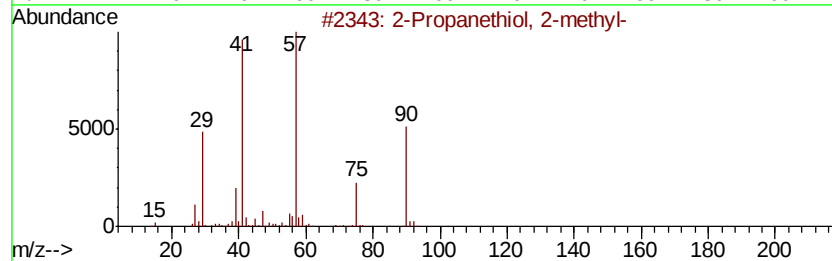
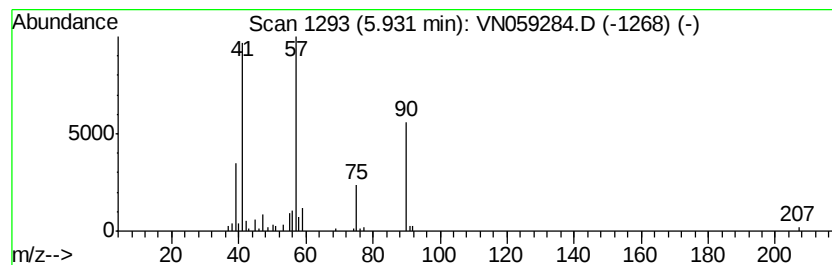
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_N\METHODS\82N110619W.M  
Quant Title : SW846 8260

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

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Peak Number 2 2-Propanethiol, 2-methyl- Concentration Rank 3

| R.T. | EstConc   | Area   | Relative to ISTD   | R.T. |
|------|-----------|--------|--------------------|------|
| 5.93 | 7.03 ug/l | 187630 | Pentafluorobenzene | 7.65 |

| Hit# | of | Tentative ID                  | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Propanethiol, 2-methyl-     | 90  | C4H10S  | 000075-66-1 | 91   |
| 2    |    | 2-Butanethiol                 | 90  | C4H10S  | 000513-53-1 | 33   |
| 3    |    | Propane, 2-methyl-2-nitro-    | 103 | C4H9NO2 | 000594-70-7 | 27   |
| 4    |    | Propanoic acid, 2,2-dimethyl- | 102 | C5H10O2 | 000075-98-9 | 25   |
| 5    |    | Ethynyl tert-butyl sulfoxide  | 130 | C6H10OS | 041463-34-7 | 25   |



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Instrument :  
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ClientSampled :  
IBLK

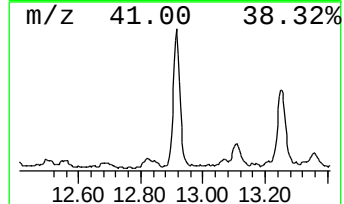
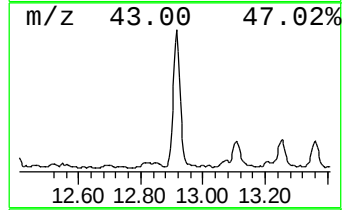
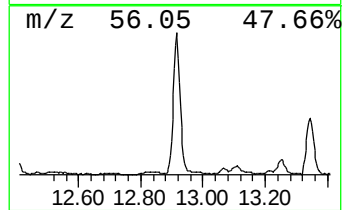
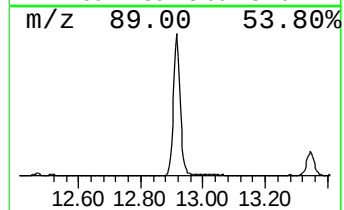
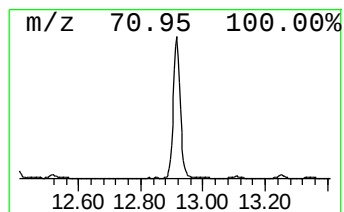
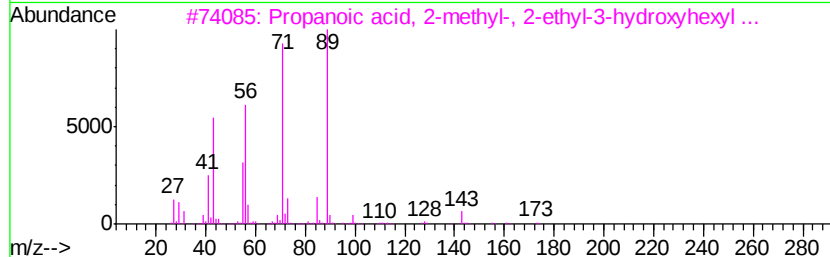
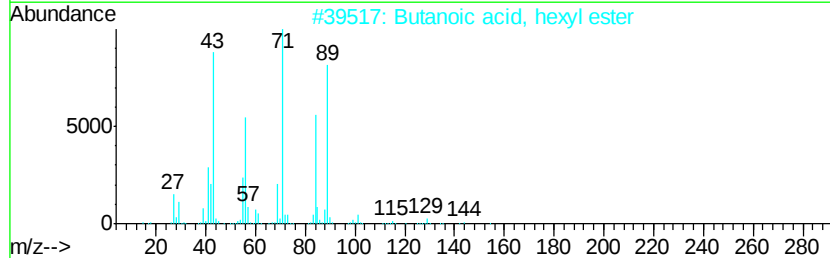
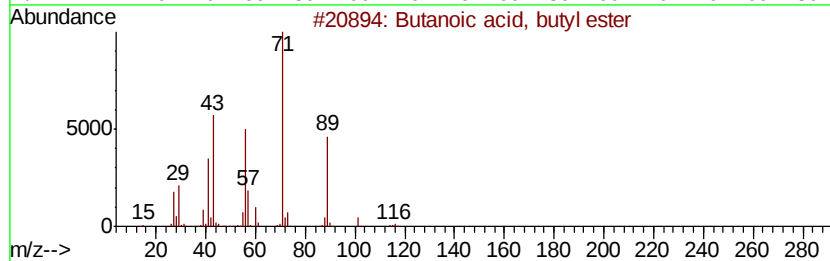
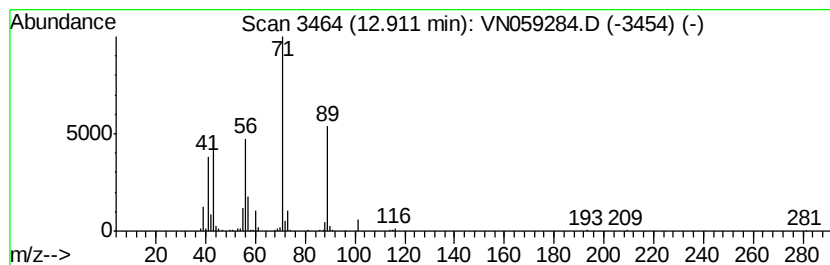
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Butanoic acid, butyl ester Concentration Rank 2

| R.T.  | EstConc   | Area   | Relative to ISTD       | R.T.  |
|-------|-----------|--------|------------------------|-------|
| 12.91 | 9.00 ug/l | 279715 | 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    |    | Propanoic acid, 2-methyl-, 2-eth... | 216 | C12H24O3 | 074367-31-0 | 64   |
| 4    |    | Butanoic acid, heptyl ester         | 186 | C11H22O2 | 005870-93-9 | 64   |
| 5    |    | Propanoic acid, 2-methyl-, 2-met... | 144 | C8H16O2  | 000097-85-8 | 45   |



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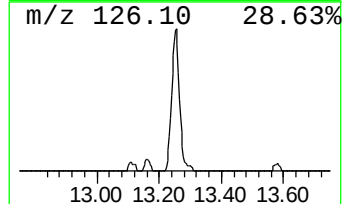
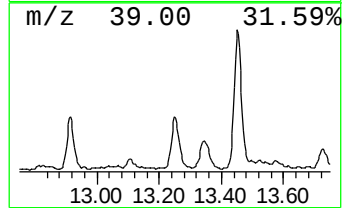
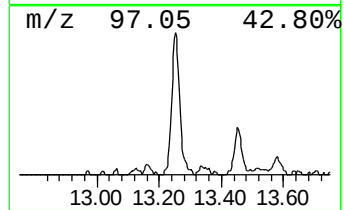
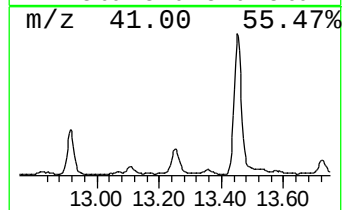
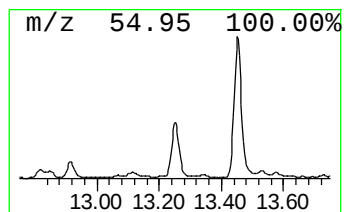
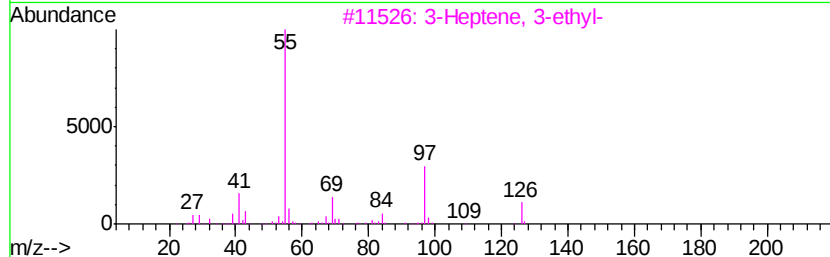
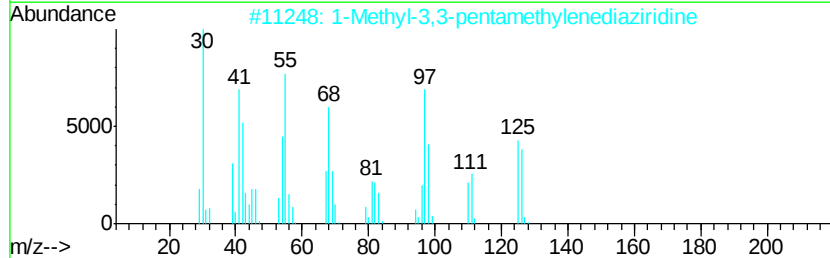
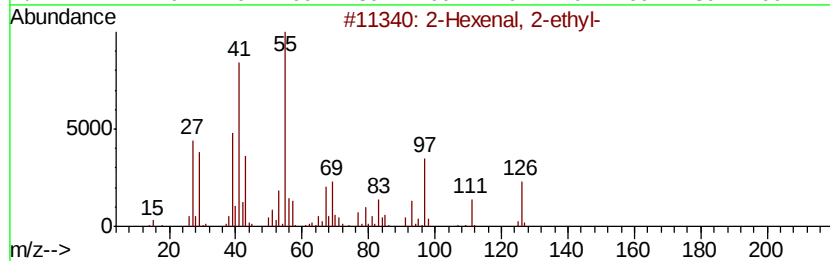
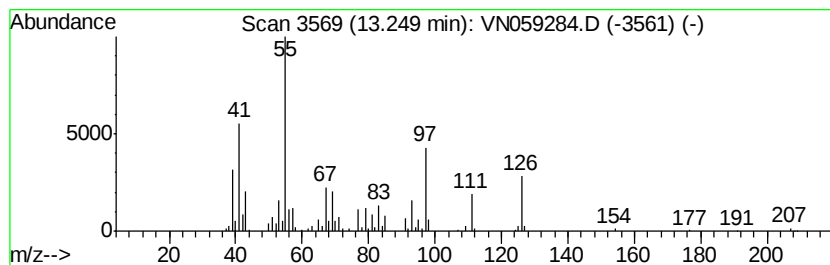
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\*\*\*\*\*  
Peak Number 4 2-Hexenal, 2-ethyl- Concentration Rank 5

| R.T.      | EstConc                             | Area   | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|--------|------------------------|-------------|------|
| 13.25     | 5.34 ug/l                           | 166107 | 1,4-Dichlorobenzene-d4 | 13.35       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm                | CAS#        | Qual |
| 1         | 2-Hexenal, 2-ethyl-                 | 126    | C8H14O                 | 000645-62-5 | 94   |
| 2         | 1-Methyl-3,3-pentamethylenediazi... | 126    | C7H14N2                | 026177-34-4 | 53   |
| 3         | 3-Heptene, 3-ethyl-                 | 126    | C9H18                  | 074764-46-8 | 47   |
| 4         | Cyclopropane, 1-bromo-2,2-diethyl-  | 176    | C7H13Br                | 343926-55-6 | 43   |
| 5         | Ethanone, 1-cyclohexyl-             | 126    | C8H14O                 | 000823-76-7 | 38   |



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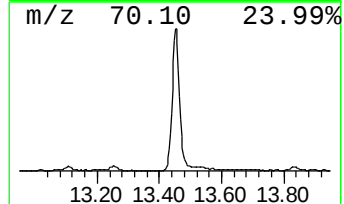
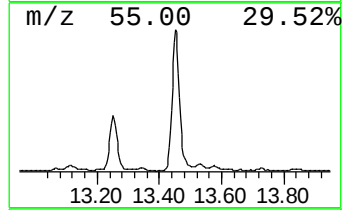
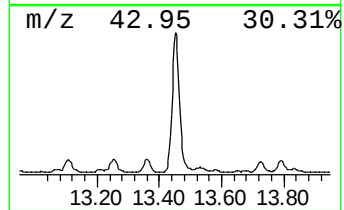
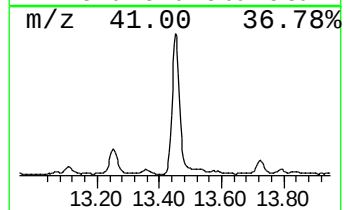
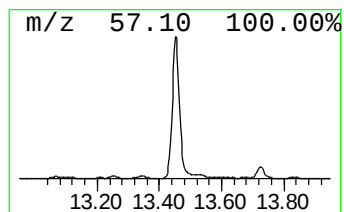
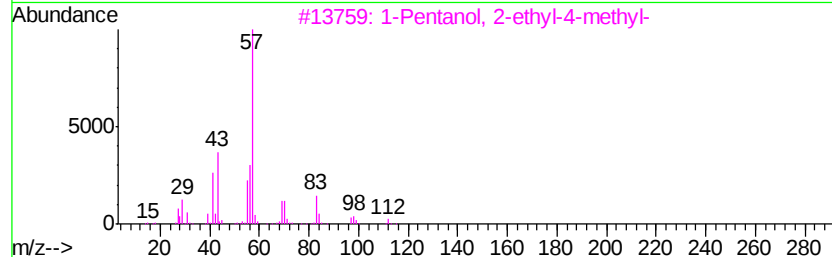
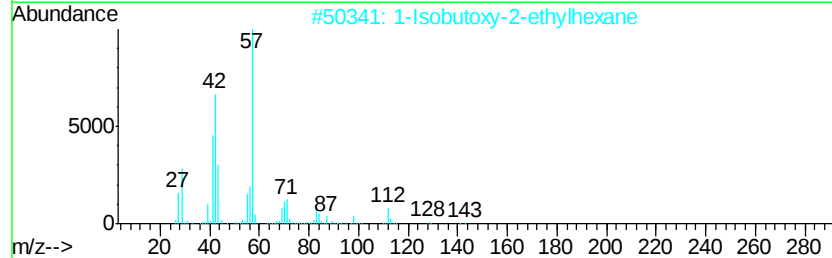
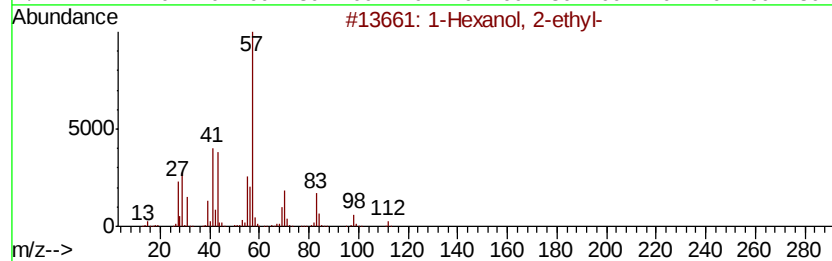
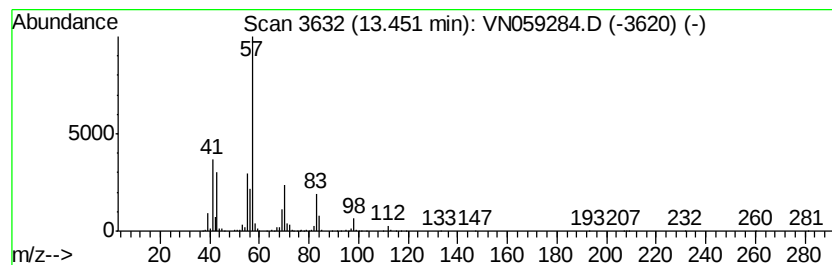
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Quant Title : SW846 8260

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

\*\*\*\*\*  
Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 1

| R.T.  | EstConc    | Area   | Relative to ISTD       | R.T.  |
|-------|------------|--------|------------------------|-------|
| 13.45 | 28.58 ug/l | 888600 | 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  | 83   |
| 2    |    | 1-Isobutoxy-2-ethylhexane           | 186 | C12H26O  | 1000139-90-3 | 56   |
| 3    |    | 1-Pentanol, 2-ethyl-4-methyl-       | 130 | C8H18O   | 000106-67-2  | 56   |
| 4    |    | 2-Propyl-1-pentanol                 | 130 | C8H18O   | 058175-57-8  | 50   |
| 5    |    | Carbonic acid, isobutyl 2-ethylh... | 230 | C13H26O3 | 1000357-82-9 | 45   |



Data Path : Z:\VOASRV\HPCHEM1\MSVOA\_N\DATA\VN111819\  
Data File : VN059284.D  
Acq On : 18 Nov 2019 15:22  
Operator : JC/SP  
Sample : IBLK  
Misc : 5.00mL/MSVOA\_N/WATER  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_N  
ClientSampleId :  
IBLK

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA\_N\METHODS\82N110619W.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 |
| 1-Propene, 2-methyl- | 2.14  | 5.4     | ug/l  | 143665   | 1                     | 7.65  | 1335360 | 50.0 |
| 2-Propanethiol, 2... | 5.93  | 7.0     | ug/l  | 187630   | 1                     | 7.65  | 1335360 | 50.0 |
| Butanoic acid, bu... | 12.91 | 9.0     | ug/l  | 279715   | 4                     | 13.35 | 1554580 | 50.0 |
| 2-Hexenal, 2-ethyl-  | 13.25 | 5.3     | ug/l  | 166107   | 4                     | 13.35 | 1554580 | 50.0 |
| 1-Hexanol, 2-ethyl-  | 13.45 | 28.6    | ug/l  | 888600   | 4                     | 13.35 | 1554580 | 50.0 |