

Data Path : Z:\VOASRV\HPCHEM1\MSVOA X\DATA\VX040620\  
 Data File : VX015508.D  
 Acq On : 06 Apr 2020 13:33  
 Operator : JC/SP  
 Sample : L2097-15 50X  
 Misc : 5.0mL/MSVOA X/WATER  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 MSVOA\_X  
 ClientSampleId :  
 40788

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\_X\METHOD\82X032720W.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         | 1.064       | 25            | 29          | 41           | rBV      | 3387430        | 3949877       | 63.14%          | 8.597%        |
| 2         | 1.472       | 92            | 96          | 104          | rVB      | 463602         | 480350        | 7.68%           | 1.045%        |
| 3         | 2.417       | 245           | 251         | 259          | rBV      | 170909         | 278755        | 4.46%           | 0.607%        |
| 4         | 2.576       | 273           | 277         | 285          | rVB      | 47295          | 83246         | 1.33%           | 0.181%        |
| 5         | 3.923       | 486           | 498         | 503          | rBV2     | 40688          | 103583        | 1.66%           | 0.225%        |
| 6         | 4.655       | 610           | 618         | 626          | rBV      | 30159          | 95449         | 1.53%           | 0.208%        |
| 7         | 5.472       | 740           | 752         | 763          | rBV      | 689424         | 1983356       | 31.71%          | 4.317%        |
| 8         | 5.630       | 768           | 778         | 793          | rVB      | 1172146        | 3270834       | 52.29%          | 7.119%        |
| 9         | 6.033       | 834           | 844         | 860          | rBV      | 779215         | 2054905       | 32.85%          | 4.472%        |
| 10        | 6.837       | 966           | 976         | 985          | rBV      | 1862755        | 4417427       | 70.62%          | 9.614%        |
| 11        | 6.941       | 985           | 993         | 1003         | rVB      | 1153295        | 2626752       | 41.99%          | 5.717%        |
| 12        | 7.270       | 1038          | 1047        | 1056         | rBV      | 663814         | 1385403       | 22.15%          | 3.015%        |
| 13        | 8.697       | 1273          | 1281        | 1300         | rBV      | 3882763        | 6160101       | 98.48%          | 13.407%       |
| 14        | 10.099      | 1505          | 1511        | 1524         | rVB      | 4196075        | 5670290       | 90.65%          | 12.341%       |
| 15        | 10.355      | 1547          | 1553        | 1562         | rBV      | 1631518        | 2201345       | 35.19%          | 4.791%        |
| 16        | 11.123      | 1674          | 1679        | 1687         | rBV      | 3811390        | 4830649       | 77.22%          | 10.514%       |
| 17        | 12.062      | 1828          | 1833        | 1841         | rVB      | 5111047        | 6255450       | 100.00%         | 13.615%       |
| 18        | 16.147      | 2499          | 2503        | 2509         | rBV5     | 53201          | 99060         | 1.58%           | 0.216%        |

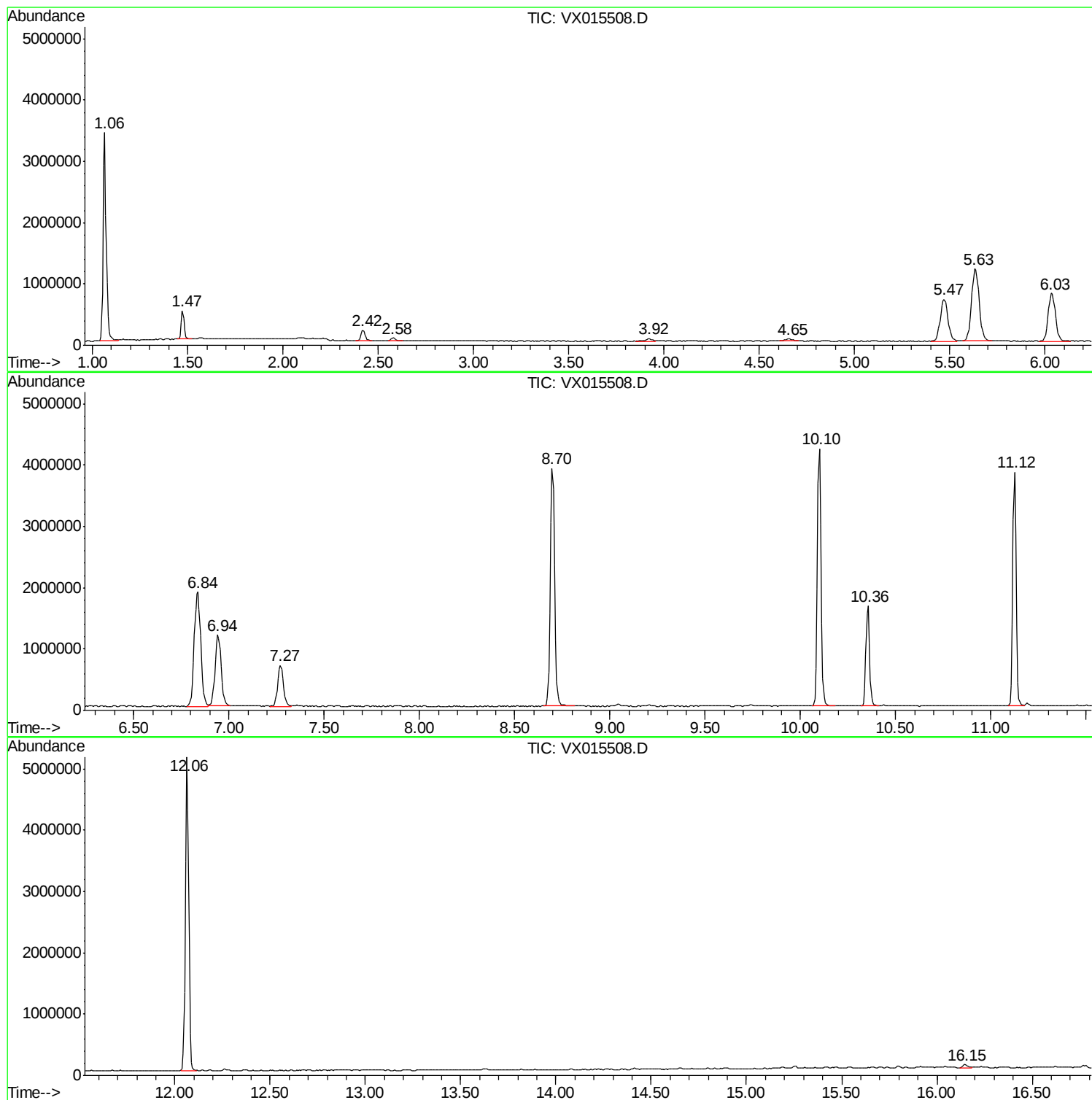
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Instrument :  
MSVOA\_X  
ClientSampleId :  
40788

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X032720W.M  
Quant Title : SW846 8260

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



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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X032720W.M  
Quant Title : SW846 8260

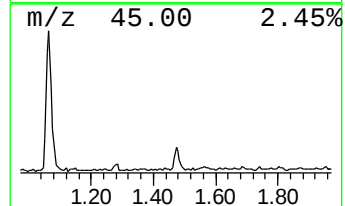
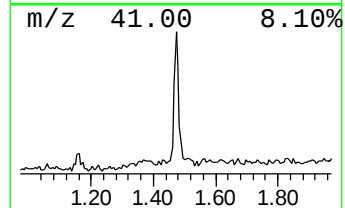
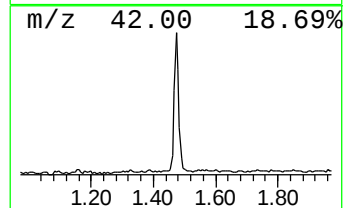
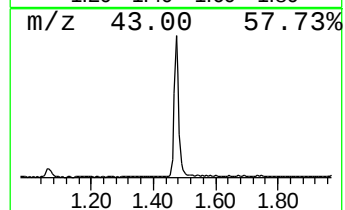
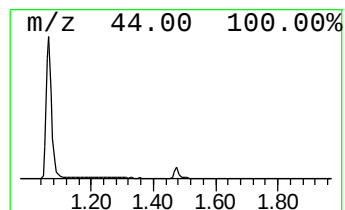
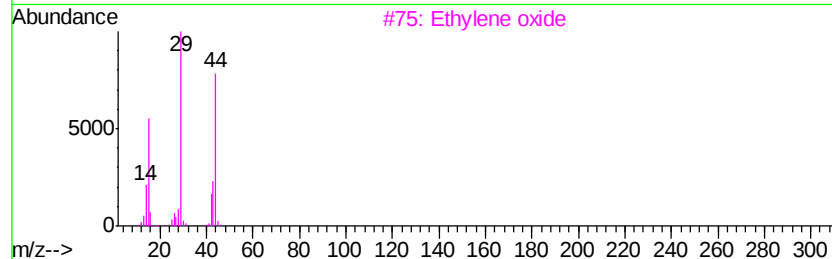
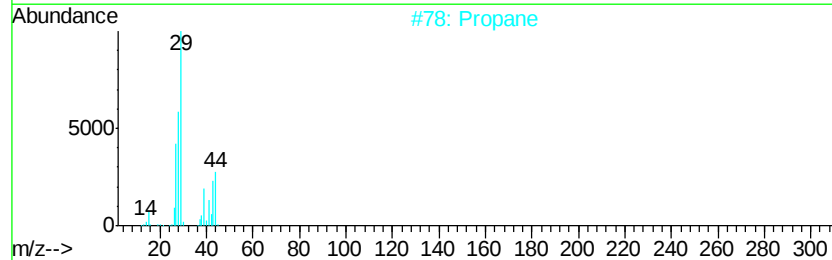
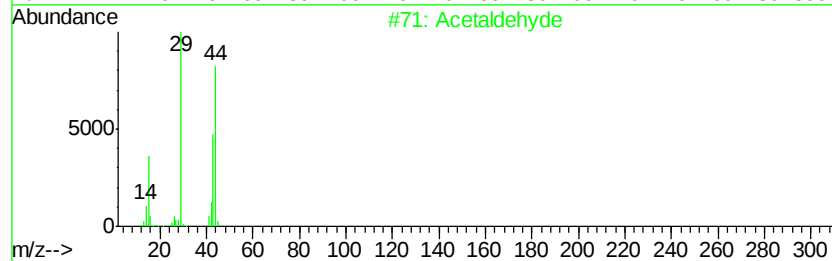
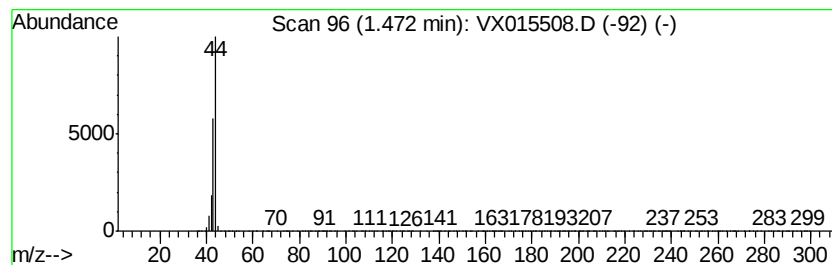
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown1.47 Concentration Rank 5

| R.T. | EstConc   | Area   | Relative to ISTD   | R.T. |
|------|-----------|--------|--------------------|------|
| 1.47 | 7.34 ug/l | 480350 | Pentafluorobenzene | 5.63 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Acetaldehydve                       | 44  | C2H4O    | 000075-07-0 | 9    |
| 2    |    | Propane                             | 44  | C3H8     | 000074-98-6 | 5    |
| 3    |    | Ethylene oxide                      | 44  | C2H4O    | 000075-21-8 | 5    |
| 4    |    | 2-Propanamine                       | 59  | C3H9N    | 000075-31-0 | 4    |
| 5    |    | Acetic acid, [(aminocarbonyl)ami... | 132 | C3H4N2O4 | 000585-05-7 | 4    |



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Instrument :  
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ClientSampleId :  
40788

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X032720W.M  
Quant Title : SW846 8260

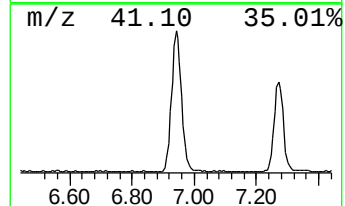
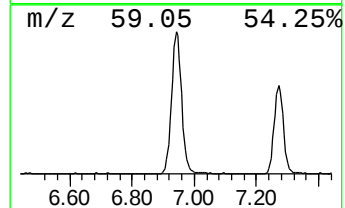
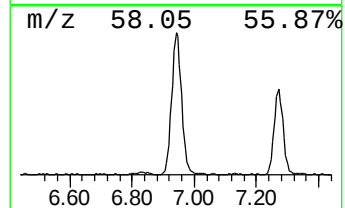
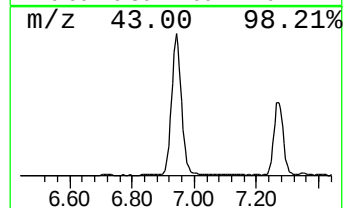
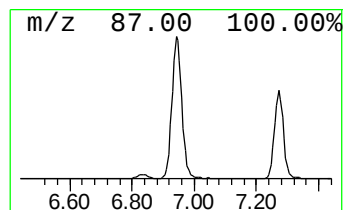
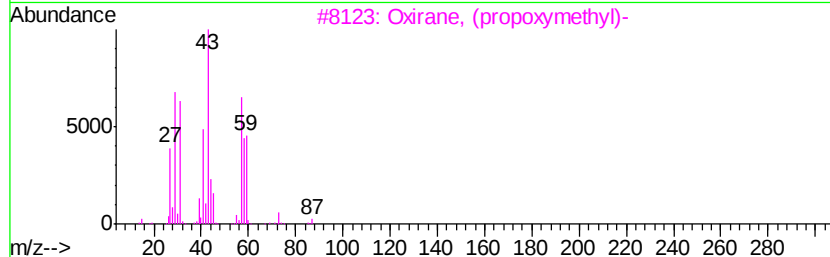
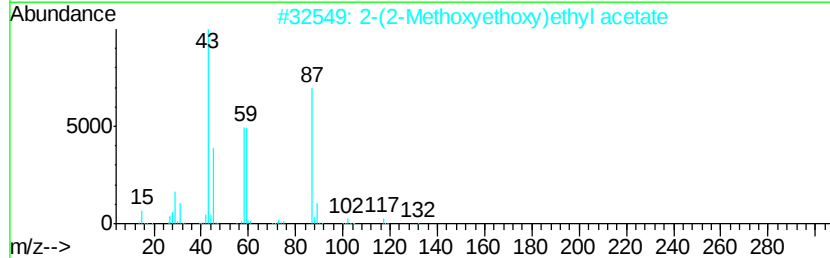
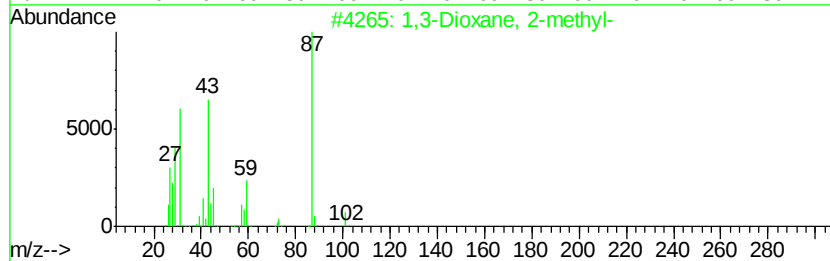
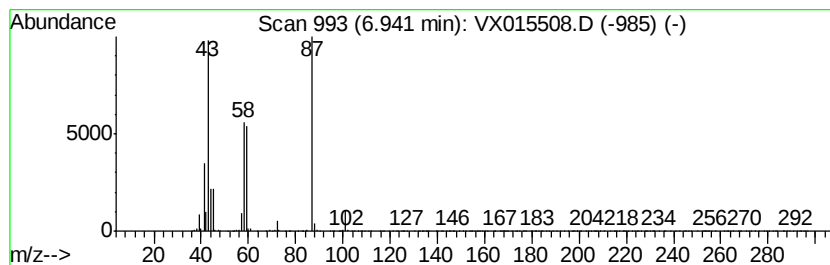
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 1,3-Dioxane, 2-methyl- Concentration Rank 2

| R.T. | EstConc    | Area    | Relative to ISTD    | R.T. |
|------|------------|---------|---------------------|------|
| 6.94 | 29.73 ug/l | 2626750 | 1,4-Difluorobenzene | 6.84 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#         | Qual |
|------|----|----------------------------------|-----|---------|--------------|------|
| 1    | 5  | 1,3-Dioxane, 2-methyl-           | 102 | C5H10O2 | 000626-68-6  | 53   |
| 2    |    | 2-(2-Methoxyethoxy)ethyl acetate | 162 | C7H14O4 | 1000351-95-4 | 45   |
| 3    |    | Oxirane, (propoxymethyl)-        | 116 | C6H12O2 | 003126-95-2  | 37   |
| 4    |    | Monomethyl malonate              | 118 | C4H6O4  | 016695-14-0  | 33   |
| 5    |    | Oxazolidin-2-one                 | 87  | C3H5NO2 | 000497-25-6  | 32   |



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ALS Vial : 9 Sample Multiplier: 1

Instrument :  
MSVOA\_X  
ClientSampleId :  
40788

Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA\_X\METHOD\82X032720W.M  
Quant Title : SW846 8260

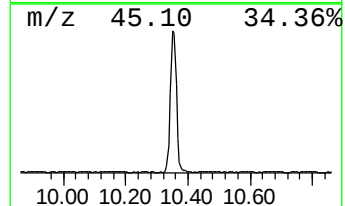
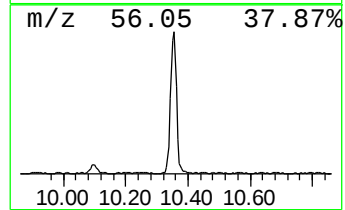
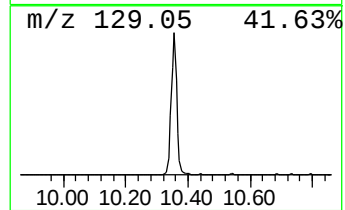
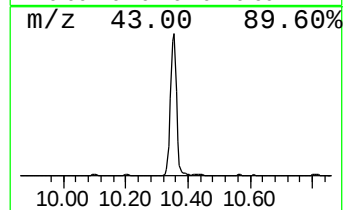
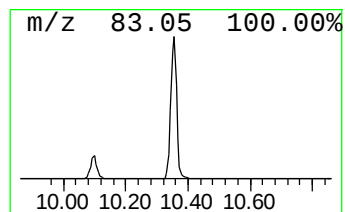
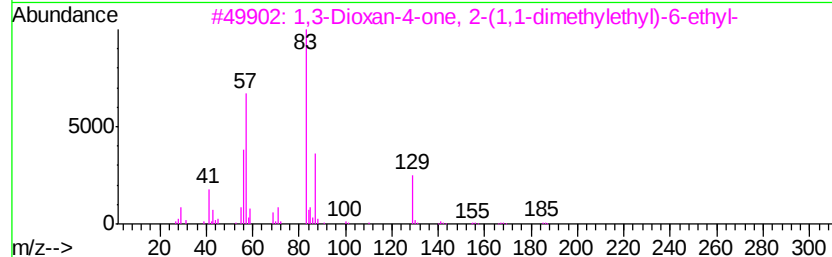
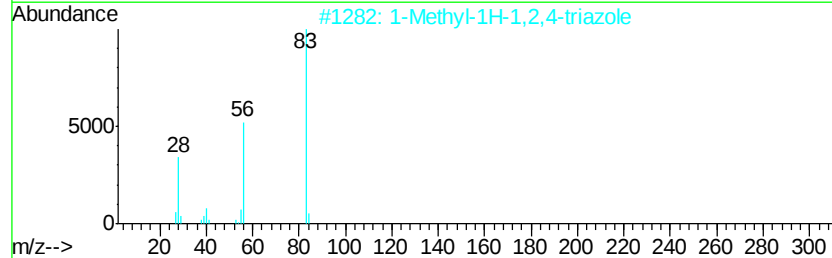
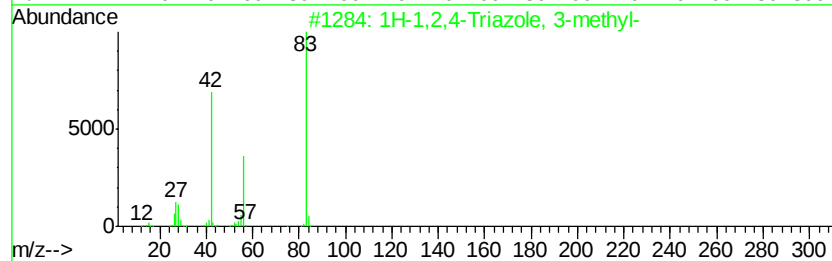
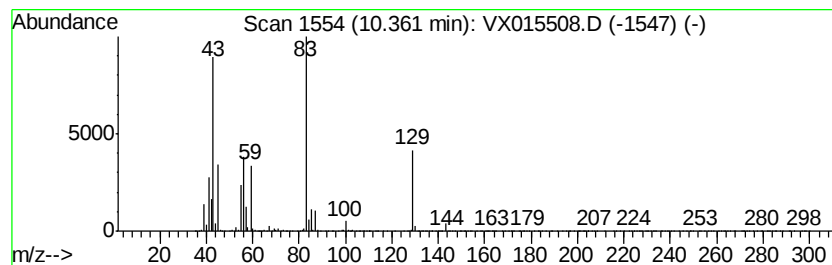
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown10.36 Concentration Rank 3

| R.T.  | EstConc    | Area    | Relative to ISTD | R.T.  |
|-------|------------|---------|------------------|-------|
| 10.36 | 19.41 ug/l | 2201350 | Chlorobenzene-d5 | 10.10 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 1H-1,2,4-Triazole, 3-methyl-        | 83  | C3H5N3    | 007170-01-6 | 25   |
| 2    |    | 1-Methyl-1H-1,2,4-triazole          | 83  | C3H5N3    | 006086-21-1 | 25   |
| 3    |    | 1,3-Dioxan-4-one, 2-(1,1-dimethv... | 186 | C10H18O3  | 113505-80-9 | 25   |
| 4    |    | 2-Butenoic acid, 2-methoxy-3-met... | 144 | C7H12O3   | 056009-32-6 | 12   |
| 5    |    | n-Hexanesulphonylacetonitrile       | 189 | C8H15NO2S | 203310-42-3 | 10   |



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ALS Vial : 9 Sample Multiplier: 1

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Quant Title : SW846 8260

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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown1.47          | 1.47  | 7.3     | ug/l  | 480350   | 1                     | 5.63  | 3270830 | 50.0 |
| 1,3-Dioxane, 2-me... | 6.94  | 29.7    | ug/l  | 2626750  | 2                     | 6.84  | 4417430 | 50.0 |
| unknown10.36         | 10.36 | 19.4    | ug/l  | 2201350  | 3                     | 10.10 | 5670290 | 50.0 |