

Data Path : Z:\voasrv\HPCHEM1\MSVOA\_Y\Data\VY091025\  
 Data File : VY023332.D  
 Acq On : 10 Sep 2025 14:49  
 Operator : SY/MD  
 Sample : Q3065-01  
 Misc : 5.00g/5.0mL/MSVOA\_Y/SOIL/A  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 MSVOA\_Y  
 ClientSampleId :  
 VNJ-204

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\_Y\methods\82Y090825S.M

Title : SW846 8260

Signal : TIC: VY023332.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         | 2.117       | 52            | 65          | 66           | rBV4     | 9083           | 31461         | 3.54%           | 0.669%        |
| 2         | 2.458       | 116           | 121         | 123          | rBV5     | 7132           | 12430         | 1.40%           | 0.264%        |
| 3         | 4.616       | 465           | 475         | 486          | rBV3     | 10412          | 31586         | 3.56%           | 0.672%        |
| 4         | 5.647       | 634           | 644         | 655          | rBV3     | 17689          | 58189         | 6.56%           | 1.238%        |
| 5         | 7.634       | 960           | 970         | 976          | rBV2     | 142761         | 334757        | 37.72%          | 7.120%        |
| 6         | 7.713       | 976           | 983         | 992          | rVB      | 226105         | 535240        | 60.30%          | 11.385%       |
| 7         | 8.061       | 1032          | 1040        | 1051         | rBV      | 100720         | 225710        | 25.43%          | 4.801%        |
| 8         | 8.615       | 1122          | 1131        | 1143         | rBV      | 339316         | 676335        | 76.20%          | 14.386%       |
| 9         | 10.109      | 1367          | 1376        | 1390         | rBV      | 507301         | 887561        | 100.00%         | 18.879%       |
| 10        | 11.414      | 1583          | 1590        | 1603         | rBV      | 417279         | 696177        | 78.44%          | 14.808%       |
| 11        | 12.407      | 1745          | 1753        | 1762         | rBV      | 257402         | 420357        | 47.36%          | 8.941%        |
| 12        | 13.346      | 1899          | 1907        | 1922         | rBV      | 289646         | 465994        | 52.50%          | 9.912%        |
| 13        | 14.206      | 2031          | 2048        | 2063         | rBV4     | 67753          | 273499        | 30.81%          | 5.817%        |
| 14        | 15.242      | 2210          | 2218        | 2228         | rBV9     | 14818          | 52093         | 5.87%           | 1.108%        |

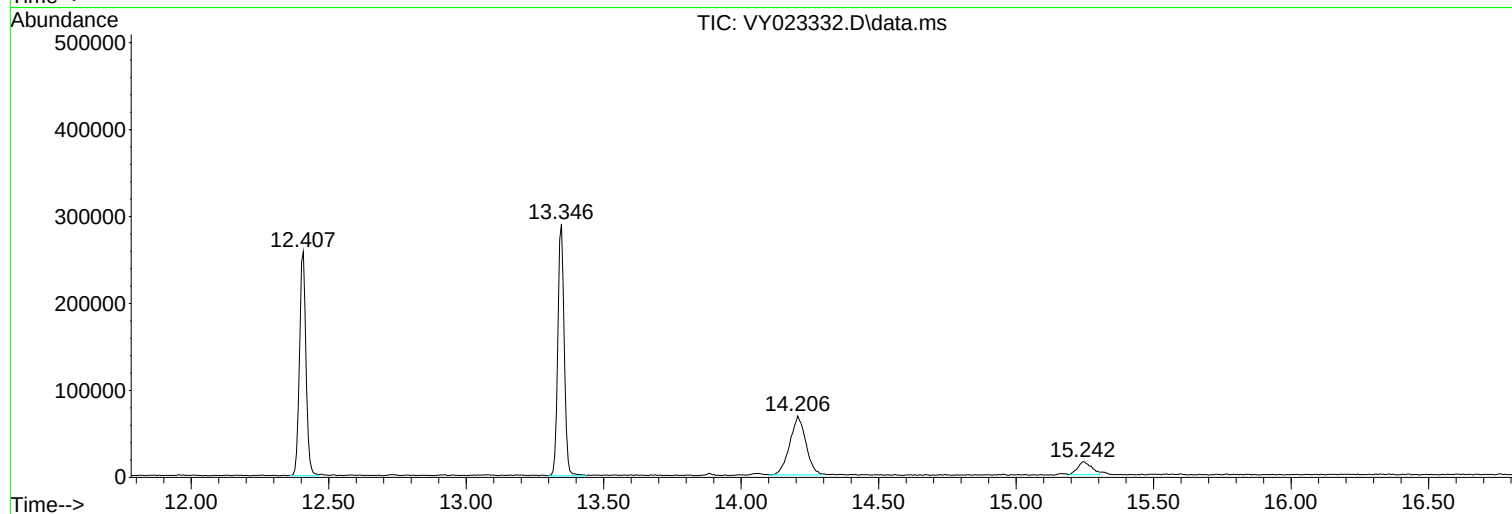
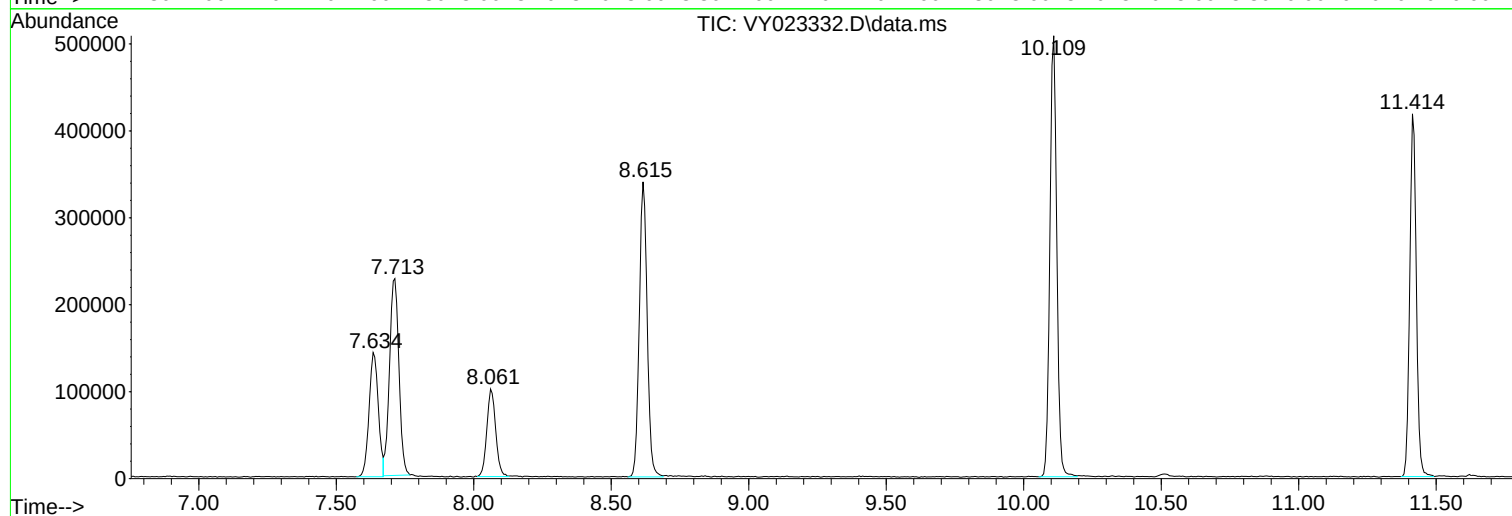
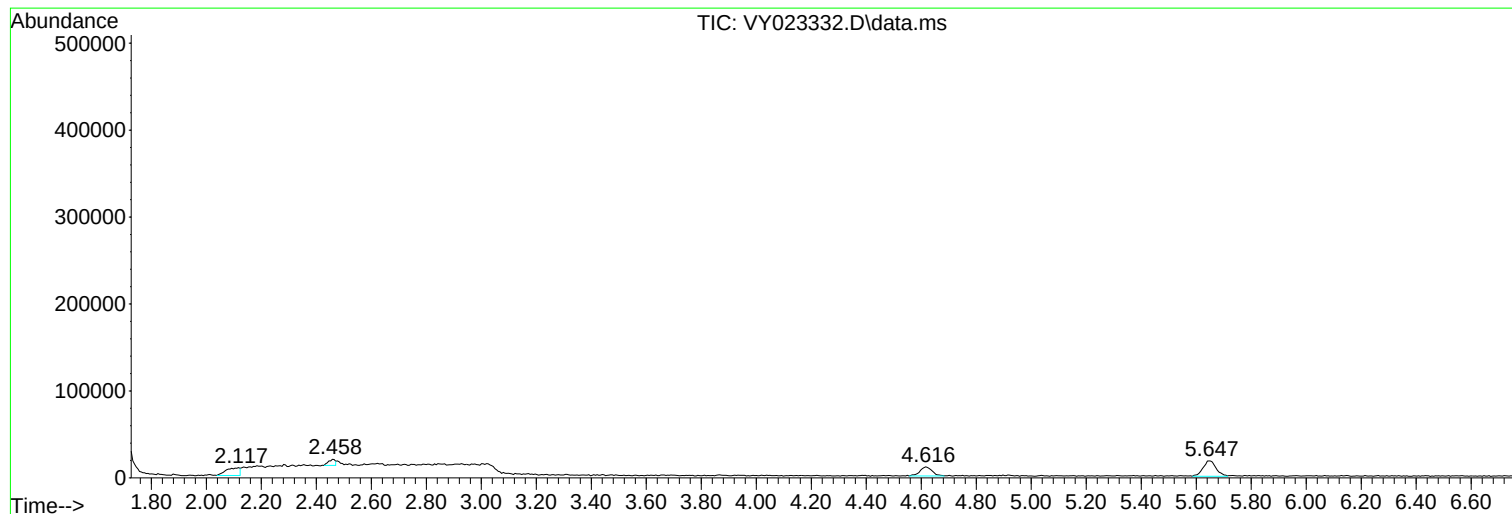
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ClientSampleId :  
VNJ-204

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090825S.M  
Quant Title : SW846 8260

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



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Quant Title : SW846 8260

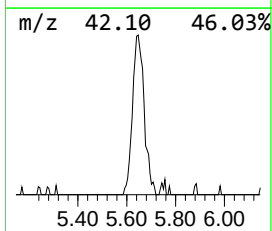
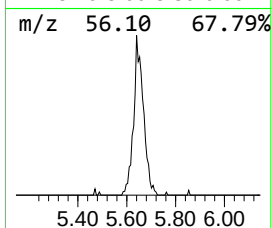
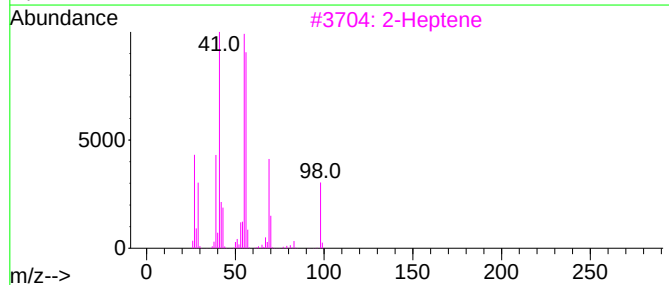
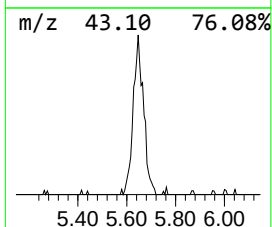
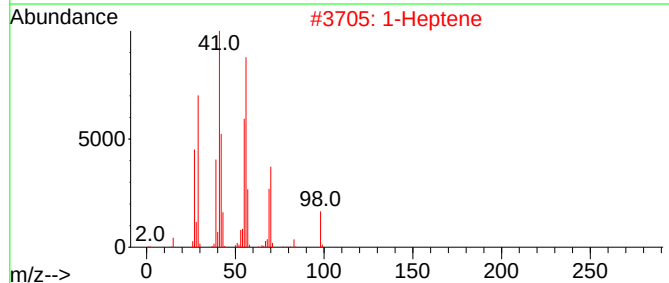
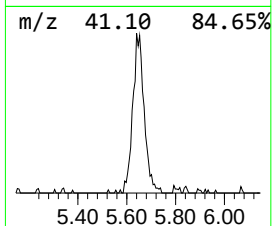
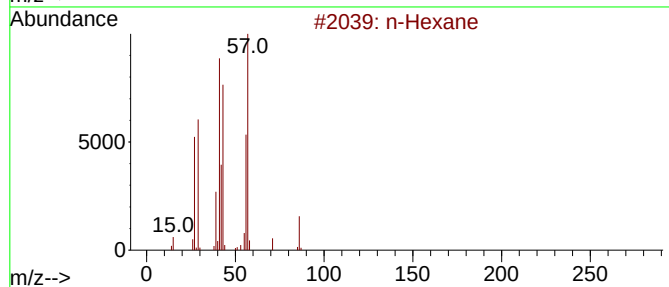
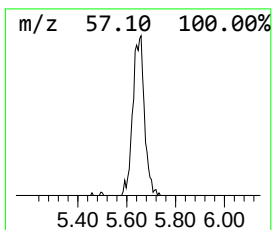
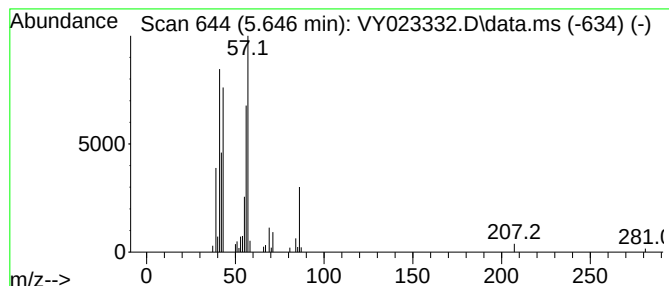
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown5.646 Concentration Rank 3

| R.T.  | EstConc   | Area  | Relative to ISTD   | R.T.  |
|-------|-----------|-------|--------------------|-------|
| 5.646 | 5.44 ug/l | 58189 | Pentafluorobenzene | 7.713 |

| Hit# | of | 5 | Tentative ID            | MW | MolForm | CAS#         | Qual |
|------|----|---|-------------------------|----|---------|--------------|------|
| 1    |    |   | n-Hexane                | 86 | C6H14   | 000110-54-3  | 47   |
| 2    |    |   | 1-Heptene               | 98 | C7H14   | 000592-76-7  | 40   |
| 3    |    |   | 2-Heptene               | 98 | C7H14   | 000592-77-8  | 38   |
| 4    |    |   | 3-Buten-1-ol, 3-methyl- | 86 | C5H10O  | 000763-32-6  | 38   |
| 5    |    |   | 2-Ethyl-oxetane         | 86 | C5H10O  | 1010386-40-2 | 38   |



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MSVOA\_Y  
ClientSampleId :  
VNJ-204

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090825S.M  
Quant Title : SW846 8260

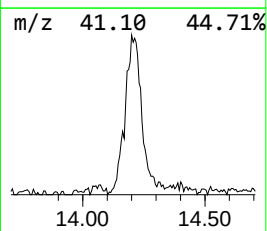
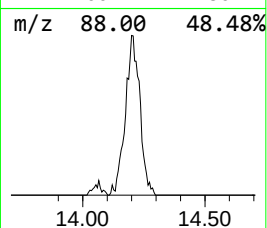
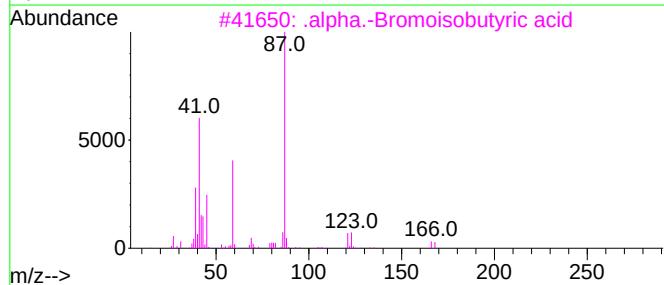
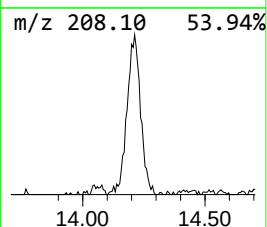
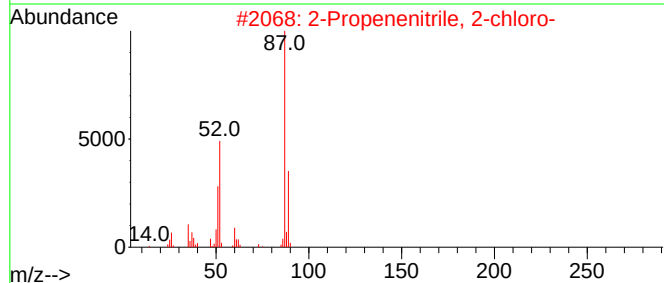
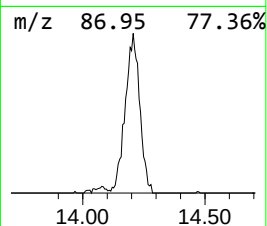
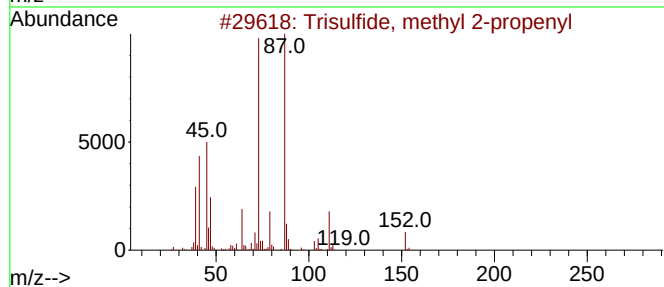
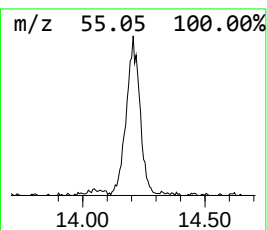
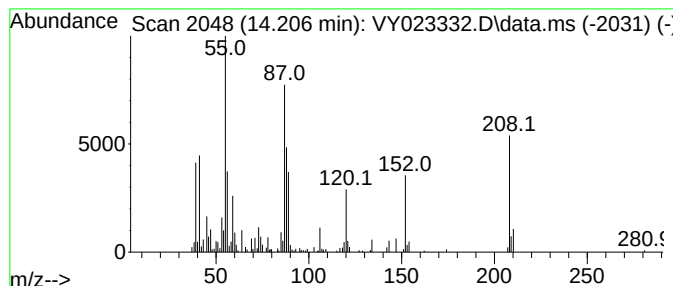
TIC Library : C:\Database\NIST20.L  
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Peak Number 2 unknown14.206 Concentration Rank 1

| R.T.   | EstConc    | Area   | Relative to ISTD       | R.T.   |
|--------|------------|--------|------------------------|--------|
| 14.206 | 29.35 ug/l | 273499 | 1,4-Dichlorobenzene-d4 | 13.346 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Trisulfide, methyl 2-propenyl       | 152 | C4H8S3   | 034135-85-8  | 35   |
| 2    |    |   | 2-Propenenitrile, 2-chloro-         | 87  | C3H2ClN  | 000920-37-6  | 27   |
| 3    |    |   | .alpha.-Bromoisobutyric acid        | 166 | C4H7BrO2 | 002052-01-9  | 22   |
| 4    |    |   | 2-[2-[2-[2-(2-Butoxyethoxy)ethox... | 336 | C16H32O7 | 1000351-94-0 | 22   |
| 5    |    |   | Thiophene, tetrahydro-2-methyl-     | 102 | C5H10S   | 001795-09-1  | 16   |



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ALS Vial : 13 Sample Multiplier: 1

Instrument :  
MSVOA\_Y  
ClientSampleId :  
VNJ-204

Quant Method : Z:\voasrv\HPCHEM1\MSVOA\_Y\methods\82Y090825S.M  
Quant Title : SW846 8260

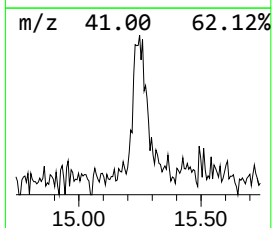
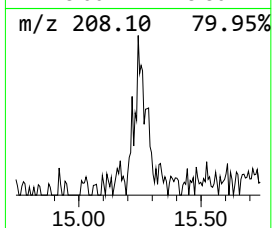
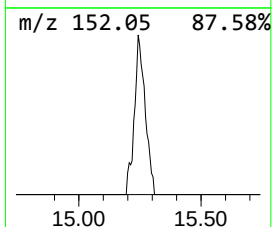
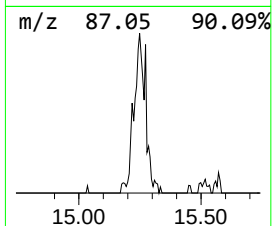
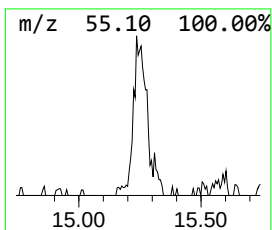
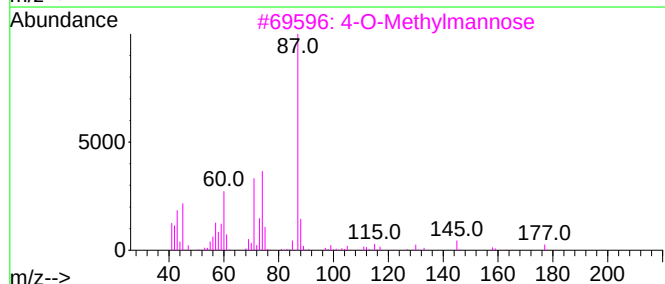
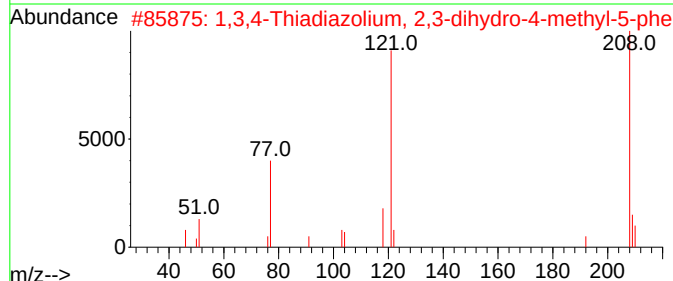
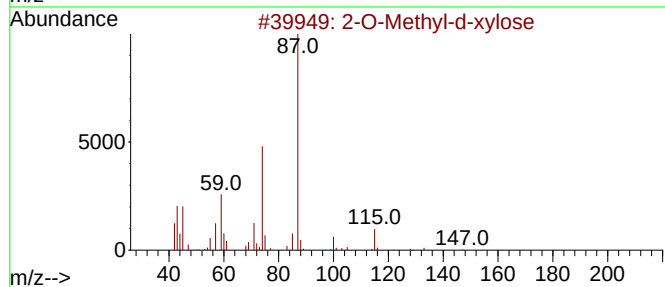
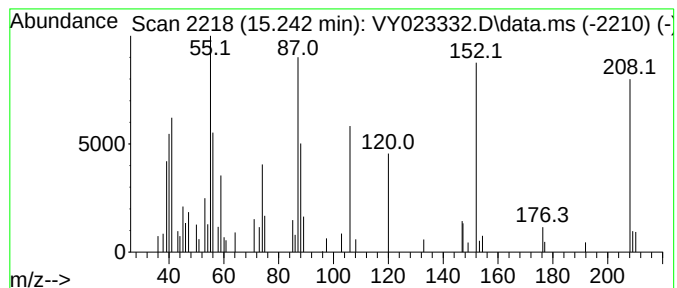
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown15.242 Concentration Rank 2

| R.T.   | EstConc   | Area  | Relative to ISTD       | R.T.   |
|--------|-----------|-------|------------------------|--------|
| 15.242 | 5.59 ug/l | 52093 | 1,4-Dichlorobenzene-d4 | 13.346 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 2-O-Methyl-d-xylose                 | 164 | C6H12O5   | 1000130-01-3 | 14   |
| 2    |    |   | 1,3,4-Thiadiazolium, 2,3-dihydro... | 208 | C9H8N2S2  | 019703-86-7  | 11   |
| 3    |    |   | 4-O-Methylmannose                   | 194 | C7H14O6   | 1000130-07-6 | 10   |
| 4    |    |   | Allyl dithioisobutyrate             | 160 | C7H12S2   | 063881-54-9  | 10   |
| 5    |    |   | 2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...    | 558 | C25H50O13 | 1000351-91-9 | 10   |



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ALS Vial : 13 Sample Multiplier: 1

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MSVOA\_Y  
ClientSampleId :  
VNJ-204

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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 |
| unknown5.646     | 5.646  | 5.4     | ug/l  | 58189    | 1                     | 7.713  | 535240 | 50.0 |
| unknown14.206    | 14.206 | 29.4    | ug/l  | 273499   | 4                     | 13.346 | 465994 | 50.0 |
| unknown15.242    | 15.242 | 5.6     | ug/l  | 52093    | 4                     | 13.346 | 465994 | 50.0 |