

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051117\  
 Data File : BM010009.D  
 Acq On : 12 May 2017 05:53  
 Operator : SJ/MA  
 Sample : I3079-07  
 Misc :  
 ALS Vial : 24 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 SS043MW039-170509

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:\HPCHEM1\BNA\_M\METHODS\8270-BM051117.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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         | 4.893       | 302           | 307         | 318          | rBV2     | 148418         | 228067        | 3.42%           | 0.863%        |
| 2         | 5.351       | 379           | 385         | 396          | rBV      | 574953         | 880310        | 13.19%          | 3.330%        |
| 3         | 5.463       | 399           | 404         | 413          | rVB      | 54972          | 92794         | 1.39%           | 0.351%        |
| 4         | 6.940       | 649           | 655         | 670          | rBV      | 345431         | 600495        | 9.00%           | 2.271%        |
| 5         | 7.293       | 708           | 715         | 725          | rBV      | 1179618        | 1912998       | 28.67%          | 7.236%        |
| 6         | 7.757       | 788           | 794         | 803          | rBV      | 247715         | 409002        | 6.13%           | 1.547%        |
| 7         | 8.075       | 841           | 848         | 859          | rBV      | 1003149        | 1677273       | 25.14%          | 6.344%        |
| 8         | 8.934       | 986           | 994         | 1006         | rBV      | 1068839        | 1792231       | 26.86%          | 6.779%        |
| 9         | 10.557      | 1260          | 1270        | 1279         | rBV      | 323309         | 566843        | 8.49%           | 2.144%        |
| 10        | 13.027      | 1682          | 1690        | 1703         | rBV      | 2457185        | 3615758       | 54.18%          | 13.677%       |
| 11        | 13.880      | 1829          | 1835        | 1844         | rBV2     | 55681          | 88567         | 1.33%           | 0.335%        |
| 12        | 14.416      | 1920          | 1926        | 1935         | rBV2     | 507939         | 789153        | 11.83%          | 2.985%        |
| 13        | 15.916      | 2175          | 2181        | 2198         | rBV      | 2234550        | 3287784       | 49.27%          | 12.436%       |
| 14        | 17.168      | 2388          | 2394        | 2405         | rBV2     | 721182         | 1075067       | 16.11%          | 4.066%        |
| 15        | 19.798      | 2835          | 2841        | 2851         | rBV      | 5526801        | 6673054       | 100.00%         | 25.241%       |
| 16        | 21.045      | 3049          | 3053        | 3062         | rBV10    | 60285          | 114620        | 1.72%           | 0.434%        |
| 17        | 21.362      | 3101          | 3107        | 3112         | rBV      | 1064802        | 1458978       | 21.86%          | 5.519%        |
| 18        | 23.650      | 3490          | 3496        | 3505         | rVB      | 566370         | 1174165       | 17.60%          | 4.441%        |

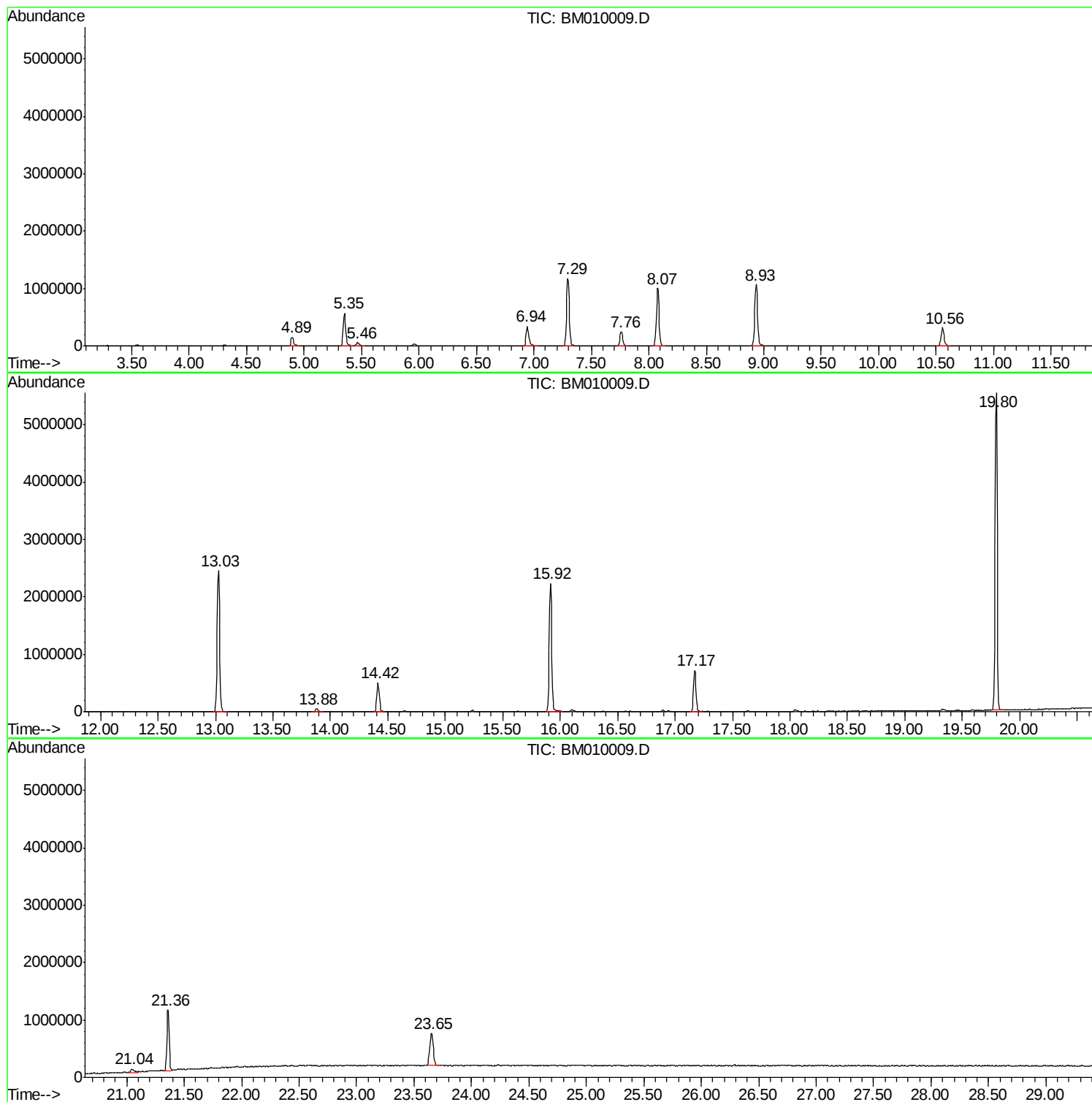
Sum of corrected areas: 26437159

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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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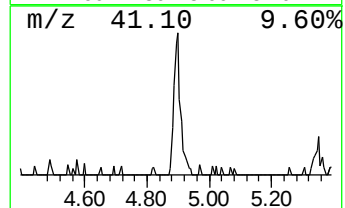
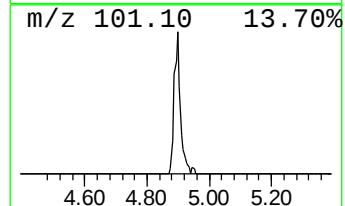
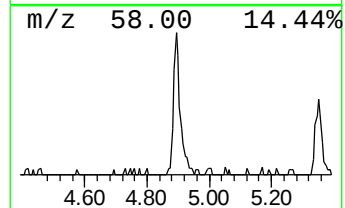
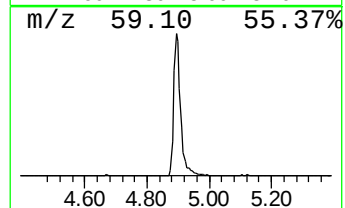
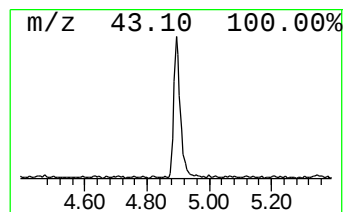
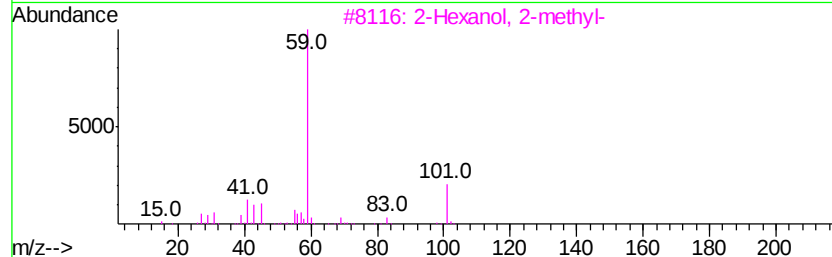
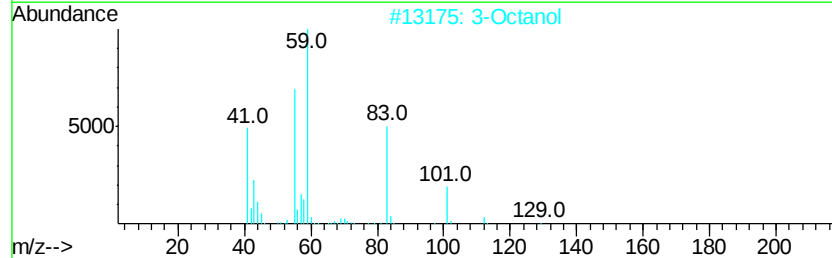
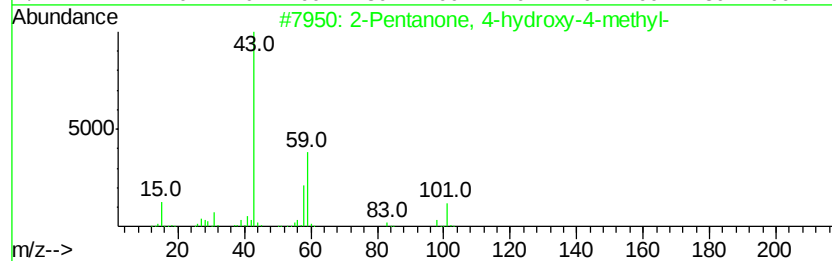
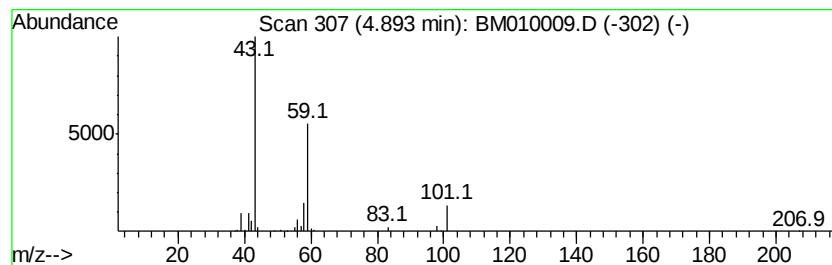
Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.89 | 11.15 ng | 228067 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-  | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    |   | 3-Octanol                         | 130 | C8H18O  | 020296-29-1 | 36   |
| 3    |    |   | 2-Hexanol, 2-methyl-              | 116 | C7H16O  | 000625-23-0 | 25   |
| 4    |    |   | 1-Propanol, 2-(2-hydroxypropoxy)- | 134 | C6H14O3 | 000106-62-7 | 23   |
| 5    |    |   | 1-Propen-2-ol, acetate            | 100 | C5H8O2  | 000108-22-5 | 10   |



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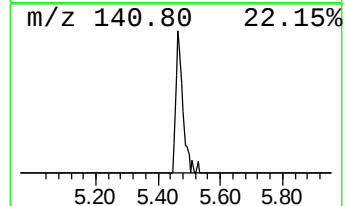
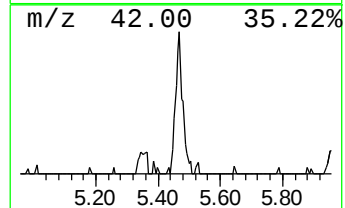
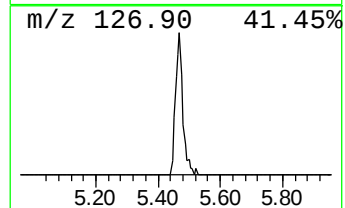
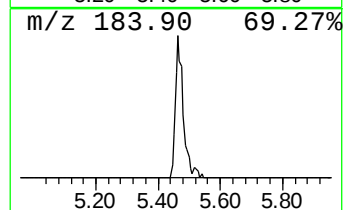
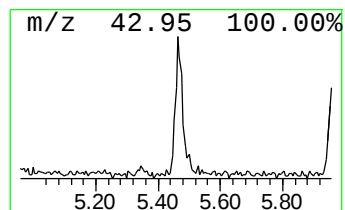
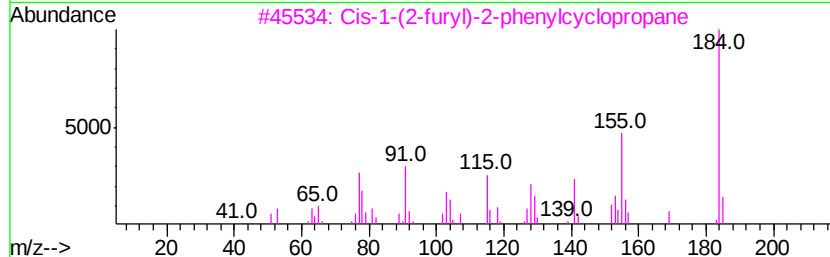
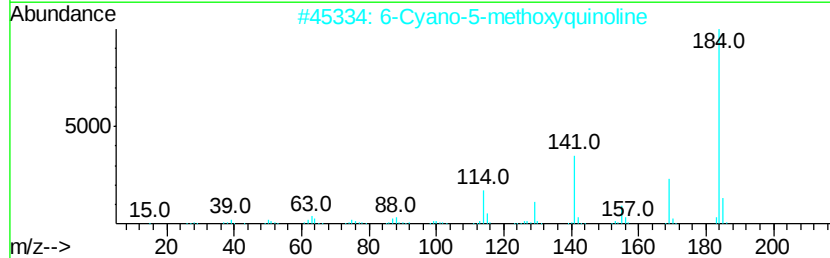
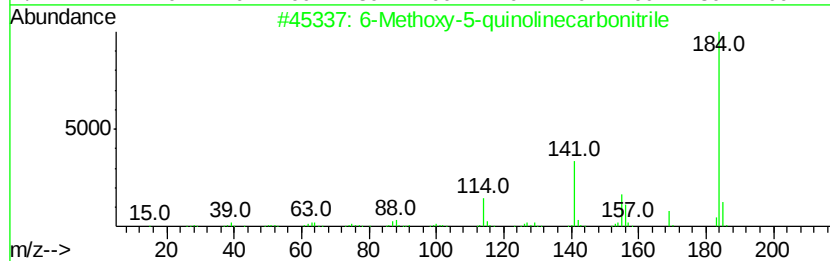
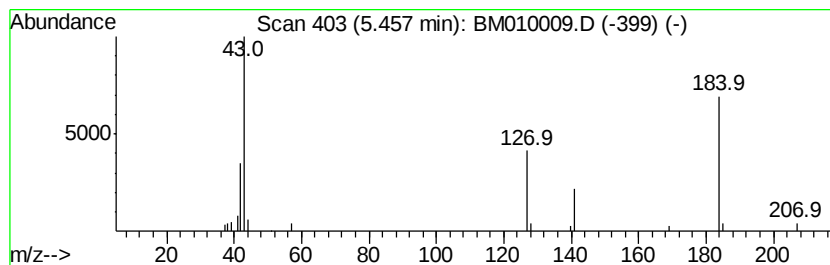
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Peak Number 2 unknown5.46 Concentration Rank 4

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.46 | 4.54 ng | 92794 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
|------|----|--------------------------------------|-----|----------|--------------|------|
| 1    | 5  | 6-Methoxy-5-quinolinecarbonitrile    | 184 | C11H8N2O | 087299-97-6  | 23   |
| 2    |    | 6-Cyano-5-methoxyquinoline           | 184 | C11H8N2O | 1000241-27-7 | 9    |
| 3    |    | Cis-1-(2-furyl)-2-phenylcyclopropane | 184 | C13H12O  | 039763-89-8  | 9    |
| 4    |    | 4H-1,3-Oxazine, 5,6-dihydro-2,4,...  | 141 | C8H15NO  | 026939-18-4  | 9    |
| 5    |    | 2-Amino-5-nitropyrimidine            | 140 | C4H4N4O2 | 003073-77-6  | 9    |



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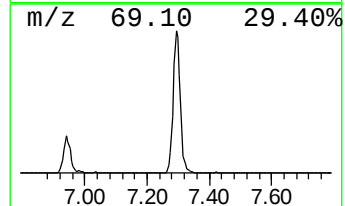
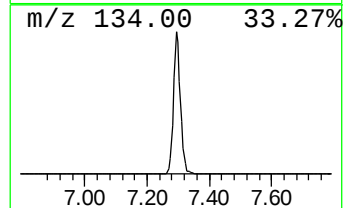
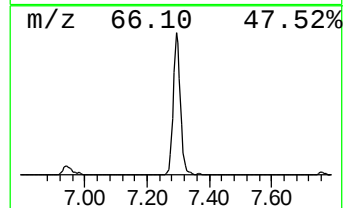
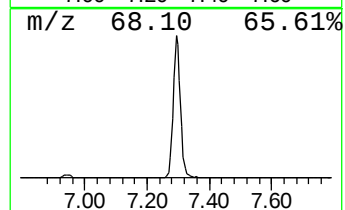
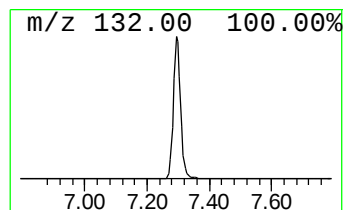
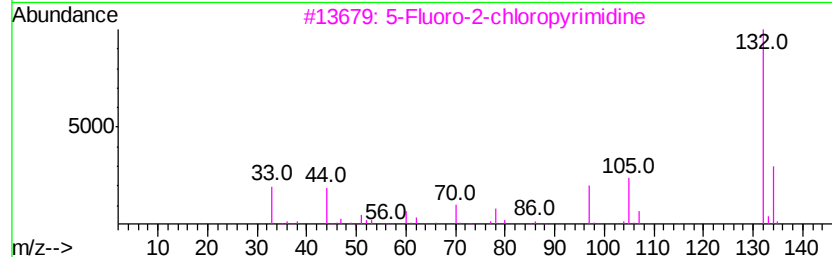
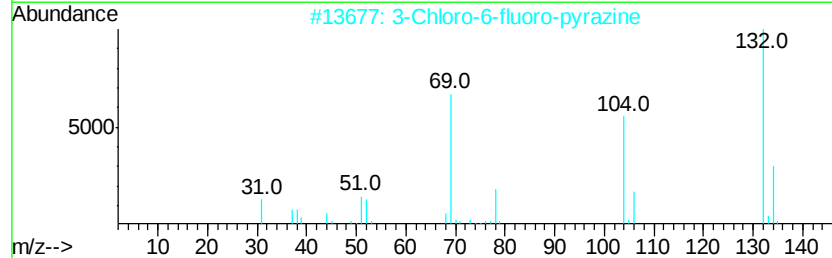
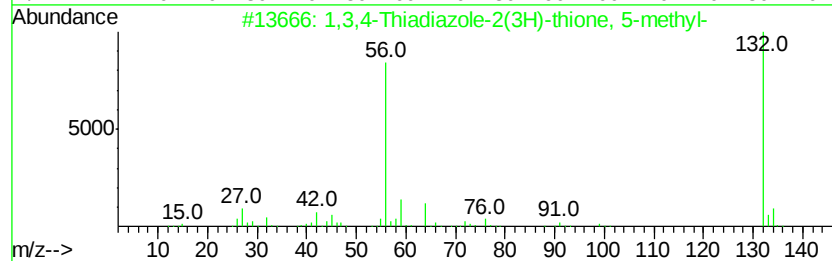
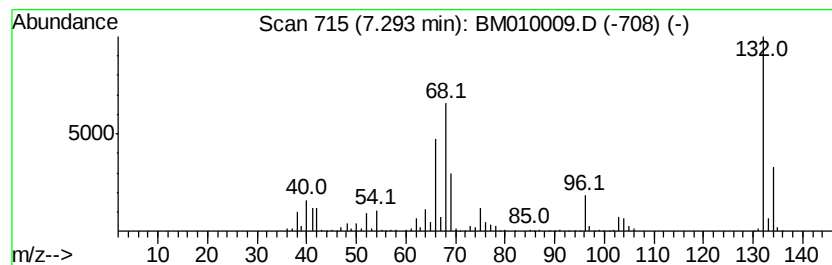
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown7.29 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.29 | 93.54 ng | 1913000 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 14   |
| 2    |    |   | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 3    |    |   | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 14   |
| 4    |    |   | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6  | 14   |
| 5    |    |   | 1,3-Cyclopentanedione, 2-chloro-    | 132 | C5H5ClO2  | 014203-19-1  | 10   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.89 | 11.2    | ng    | 228067   | 1                     | 7.76 | 409002 | 20.0 |
| unknown5.46          | 5.46 | 4.5     | ng    | 92794    | 1                     | 7.76 | 409002 | 20.0 |
| unknown7.29          | 7.29 | 93.5    | ng    | 1913000  | 1                     | 7.76 | 409002 | 20.0 |