

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF021517\  
 Data File : BF092957.D  
 Acq On : 15 Feb 2017 18:08  
 Operator : SJ/MA  
 Sample : I1835-05  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TEST-PIT-3-COMP

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\_F\METHODS\8270-BF013017.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         | 2.658       | 49            | 50          | 56           | rVB      | 129512         | 215144        | 4.40%           | 0.554%        |
| 2         | 5.059       | 257           | 260         | 268          | rBV      | 1340290        | 1900284       | 38.90%          | 4.895%        |
| 3         | 5.482       | 294           | 297         | 299          | rBV      | 3514479        | 4012875       | 82.15%          | 10.337%       |
| 4         | 6.510       | 384           | 387         | 390          | rBV      | 3203704        | 3355564       | 68.69%          | 8.644%        |
| 5         | 6.647       | 396           | 399         | 401          | rBV      | 3288719        | 4191336       | 85.80%          | 10.797%       |
| 6         | 6.876       | 416           | 419         | 421          | rBV      | 721309         | 845467        | 17.31%          | 2.178%        |
| 7         | 7.025       | 430           | 432         | 435          | rBV      | 2581013        | 2921128       | 59.80%          | 7.525%        |
| 8         | 7.436       | 465           | 468         | 471          | rBV      | 2287870        | 2469320       | 50.55%          | 6.361%        |
| 9         | 8.156       | 528           | 531         | 533          | rBV      | 1405142        | 1217942       | 24.93%          | 3.137%        |
| 10        | 9.230       | 622           | 625         | 628          | rBV      | 4265504        | 4351516       | 89.08%          | 11.209%       |
| 11        | 9.825       | 669           | 677         | 682          | rBV      | 101204         | 215158        | 4.40%           | 0.554%        |
| 12        | 9.905       | 682           | 684         | 686          | rVB      | 1596310        | 1366577       | 27.98%          | 3.520%        |
| 13        | 10.694      | 750           | 753         | 756          | rBV      | 2337195        | 2684878       | 54.96%          | 6.916%        |
| 14        | 11.391      | 811           | 814         | 816          | rBV      | 1482241        | 1417093       | 29.01%          | 3.650%        |
| 15        | 12.728      | 928           | 931         | 933          | rBV      | 197767         | 255363        | 5.23%           | 0.658%        |
| 16        | 12.979      | 950           | 953         | 955          | rBV      | 4263518        | 4884937       | 100.00%         | 12.583%       |
| 17        | 14.020      | 1042          | 1044        | 1047         | rVB      | 1372510        | 1317276       | 26.97%          | 3.393%        |
| 18        | 15.460      | 1167          | 1170        | 1179         | rVB      | 906784         | 1198979       | 24.54%          | 3.088%        |

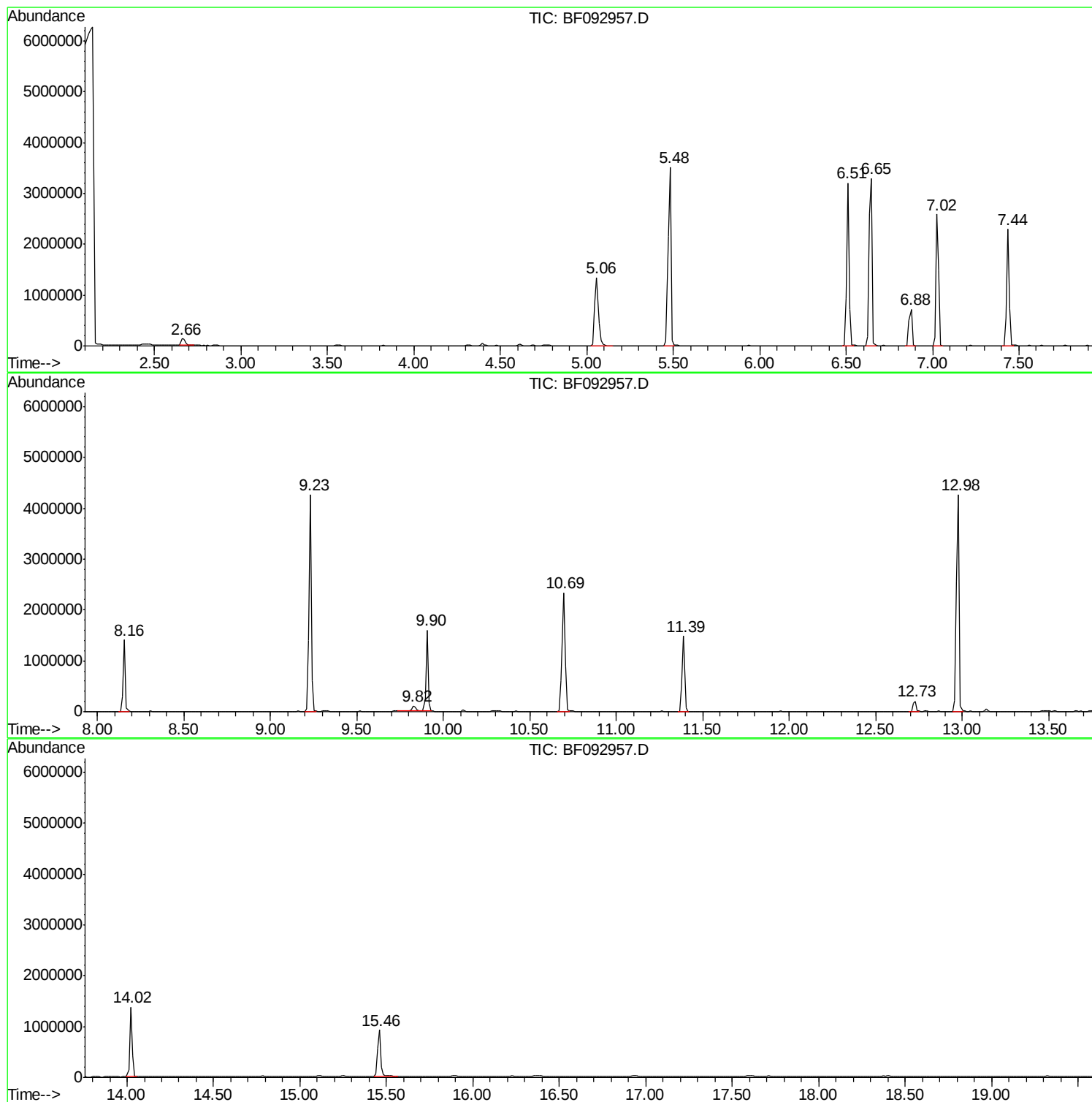
Sum of corrected areas: 38820837

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



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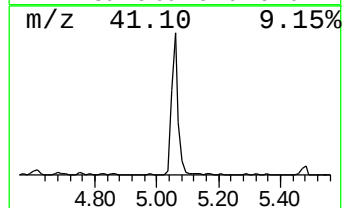
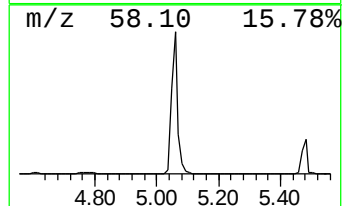
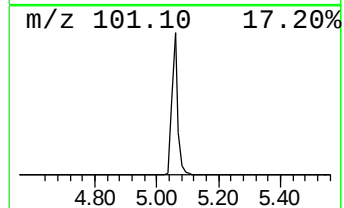
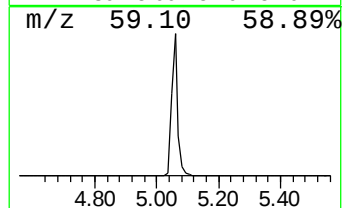
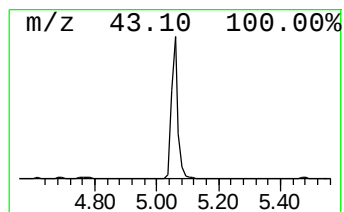
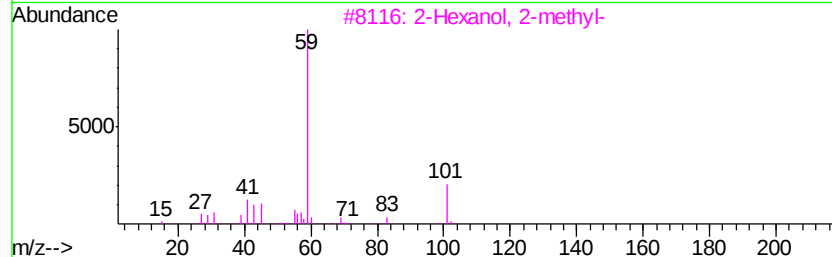
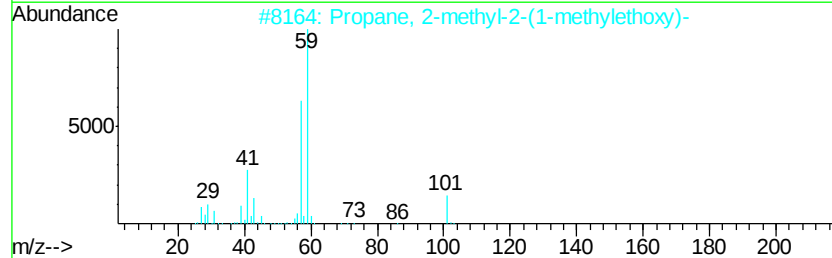
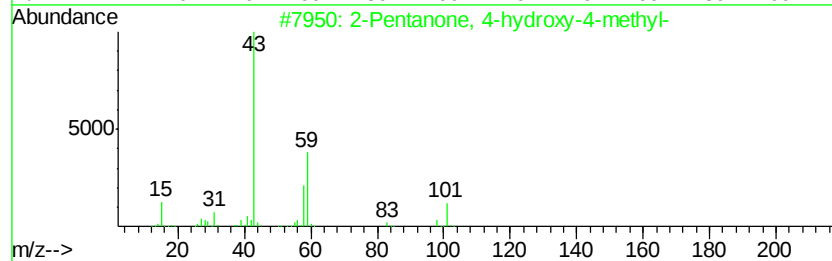
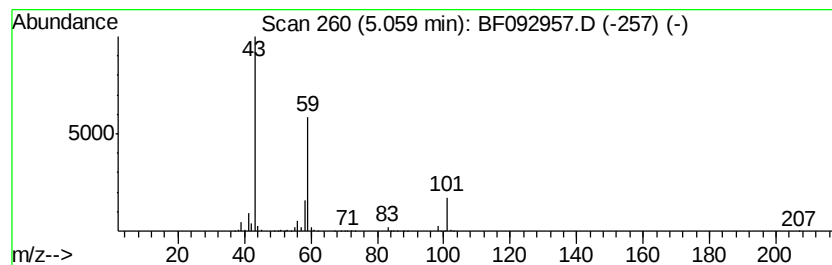
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 5.06 | 44.95 ng | 1900280 | 1,4-Dichlorobenzene-d4 | 6.88 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 33   |
| 3    |    | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 4    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 5    |    | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 10   |



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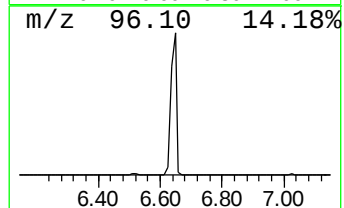
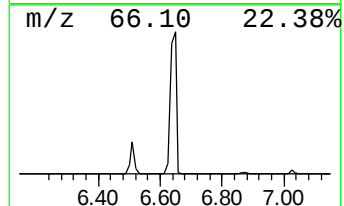
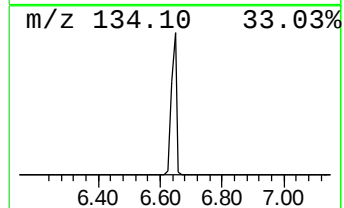
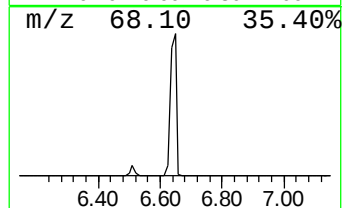
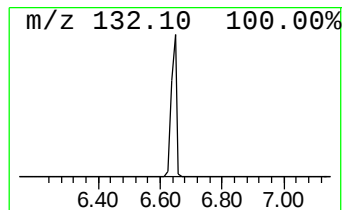
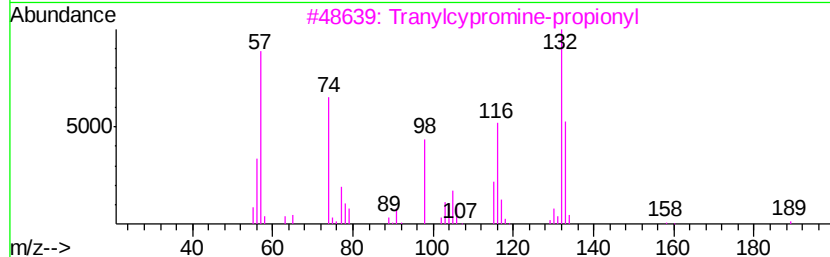
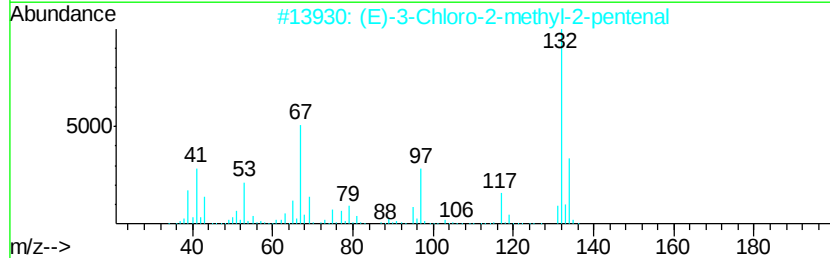
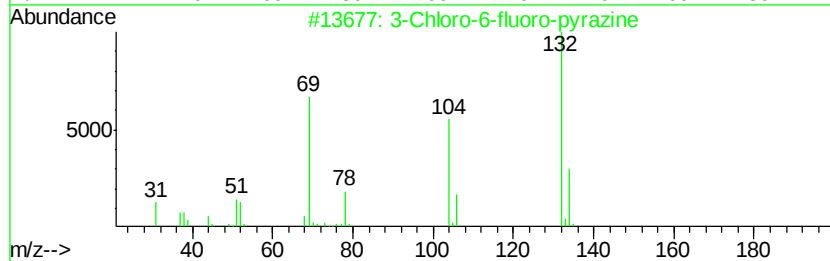
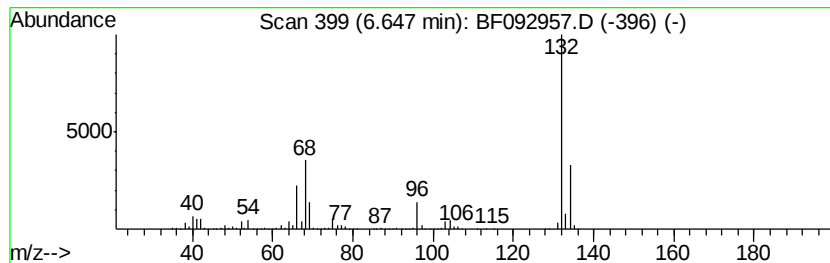
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Peak Number 3 unknown6.65 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.65 | 99.15 ng | 4191340 | 1,4-Dichlorobenzene-d4 | 6.88 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 38   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 16   |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 5    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |



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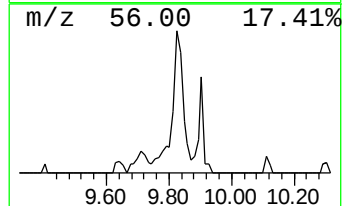
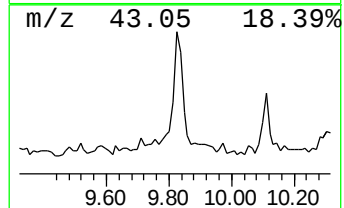
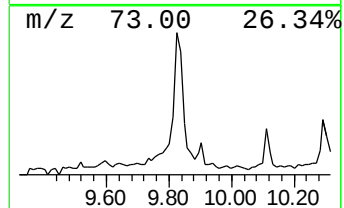
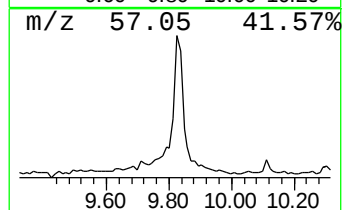
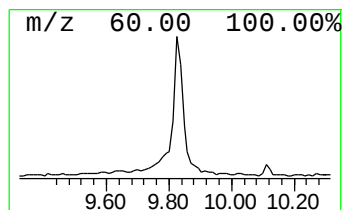
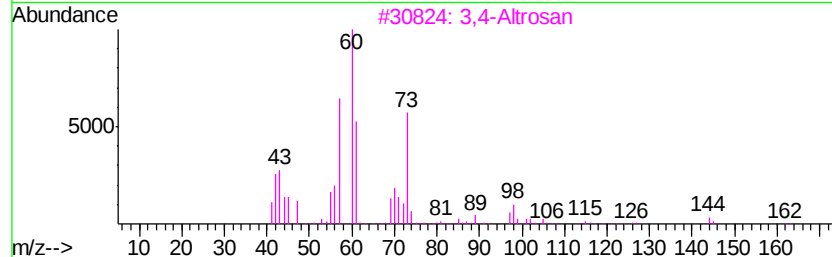
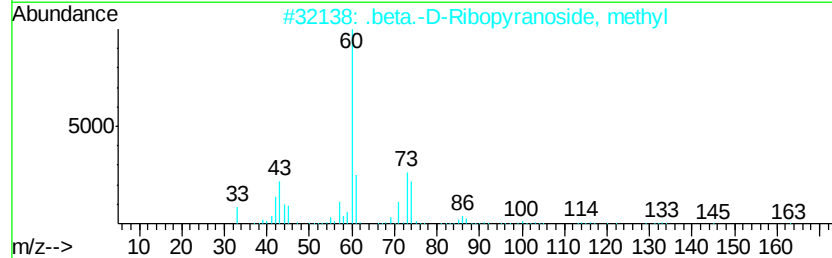
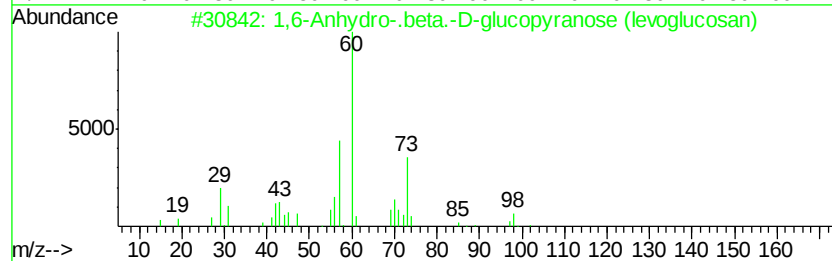
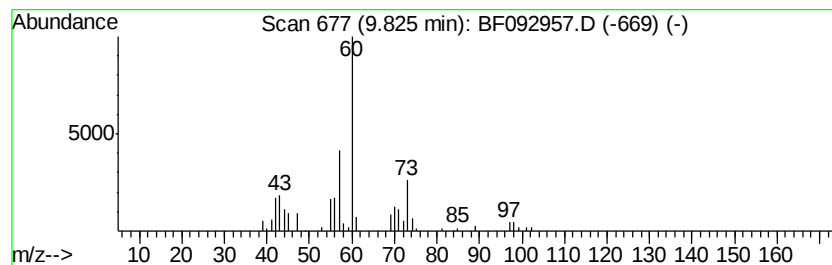
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Peak Number 5 1,6-Anhydro-.beta.-D-glucop... Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.82 | 3.15 ng | 215158 | Acenaphthene-d10 | 9.90 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|---------|---|-------------------------------------|-----|-----------|--------------|------|
| 1       |   | 1,6-Anhydro-.beta.-D-glucopyrano... | 162 | C6H10O5   | 000498-07-7  | 72   |
| 2       |   | .beta.-D-Ribopyranoside, methyl     | 164 | C6H12O5   | 017289-61-1  | 45   |
| 3       |   | 3,4-Altrosan                        | 162 | C6H10O5   | 1000129-76-4 | 40   |
| 4       |   | Hexanoic acid                       | 116 | C6H12O2   | 000142-62-1  | 36   |
| 5       |   | Hexanoic acid, 6-bromo-             | 194 | C6H11BrO2 | 004224-70-8  | 33   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |         |      |
|----------------------|------|---------|-------|----------|-----------------------|------|---------|------|
|                      |      |         |       |          | #                     | RT   | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.06 | 45.0    | ng    | 1900280  | 1                     | 6.88 | 845467  | 20.0 |
| unknown6.65          | 6.65 | 99.2    | ng    | 4191340  | 1                     | 6.88 | 845467  | 20.0 |
| 1,6-Anhydro-.beta... | 9.82 | 3.1     | ng    | 215158   | 3                     | 9.90 | 1366580 | 20.0 |