

Data Path : Z:\HPCHEM1\BNA\_M\DATA\BM050617\  
 Data File : BM009952.D  
 Acq On : 06 May 2017 22:03  
 Operator : SJ/MA  
 Sample : I2992-01  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 R1-MW-3-GW

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-BM050517.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         | 4.904       | 304           | 309         | 317          | rBV      | 137010         | 194595        | 2.54%           | 0.497%        |
| 2         | 5.363       | 381           | 387         | 398          | rBV      | 1354374        | 2019167       | 26.40%          | 5.152%        |
| 3         | 6.957       | 651           | 658         | 674          | rBV      | 852811         | 1402044       | 18.33%          | 3.577%        |
| 4         | 7.310       | 711           | 718         | 732          | rBV      | 2311210        | 3668938       | 47.98%          | 9.362%        |
| 5         | 7.769       | 789           | 796         | 805          | rBV      | 427994         | 697474        | 9.12%           | 1.780%        |
| 6         | 8.087       | 841           | 850         | 859          | rBV      | 1896099        | 3091627       | 40.43%          | 7.889%        |
| 7         | 8.945       | 988           | 996         | 1008         | rBV      | 1856065        | 3072183       | 40.17%          | 7.839%        |
| 8         | 10.569      | 1265          | 1272        | 1284         | rBV      | 533484         | 921875        | 12.05%          | 2.352%        |
| 9         | 13.039      | 1685          | 1692        | 1701         | rBV      | 4194952        | 5846914       | 76.46%          | 14.919%       |
| 10        | 14.427      | 1921          | 1928        | 1934         | rBV2     | 748064         | 1128663       | 14.76%          | 2.880%        |
| 11        | 14.827      | 1992          | 1996        | 2003         | rVB      | 51512          | 88364         | 1.16%           | 0.225%        |
| 12        | 15.927      | 2177          | 2183        | 2194         | rBV      | 3579305        | 5081918       | 66.45%          | 12.967%       |
| 13        | 17.180      | 2388          | 2396        | 2404         | rBV      | 996028         | 1454982       | 19.03%          | 3.712%        |
| 14        | 17.604      | 2463          | 2468        | 2473         | rBV      | 88755          | 123475        | 1.61%           | 0.315%        |
| 15        | 19.809      | 2837          | 2843        | 2848         | rBV      | 6436935        | 7647488       | 100.00%         | 19.513%       |
| 16        | 21.368      | 3104          | 3108        | 3114         | rBV      | 1173549        | 1524691       | 19.94%          | 3.890%        |
| 17        | 23.674      | 3494          | 3500        | 3506         | rVB      | 667157         | 1227169       | 16.05%          | 3.131%        |

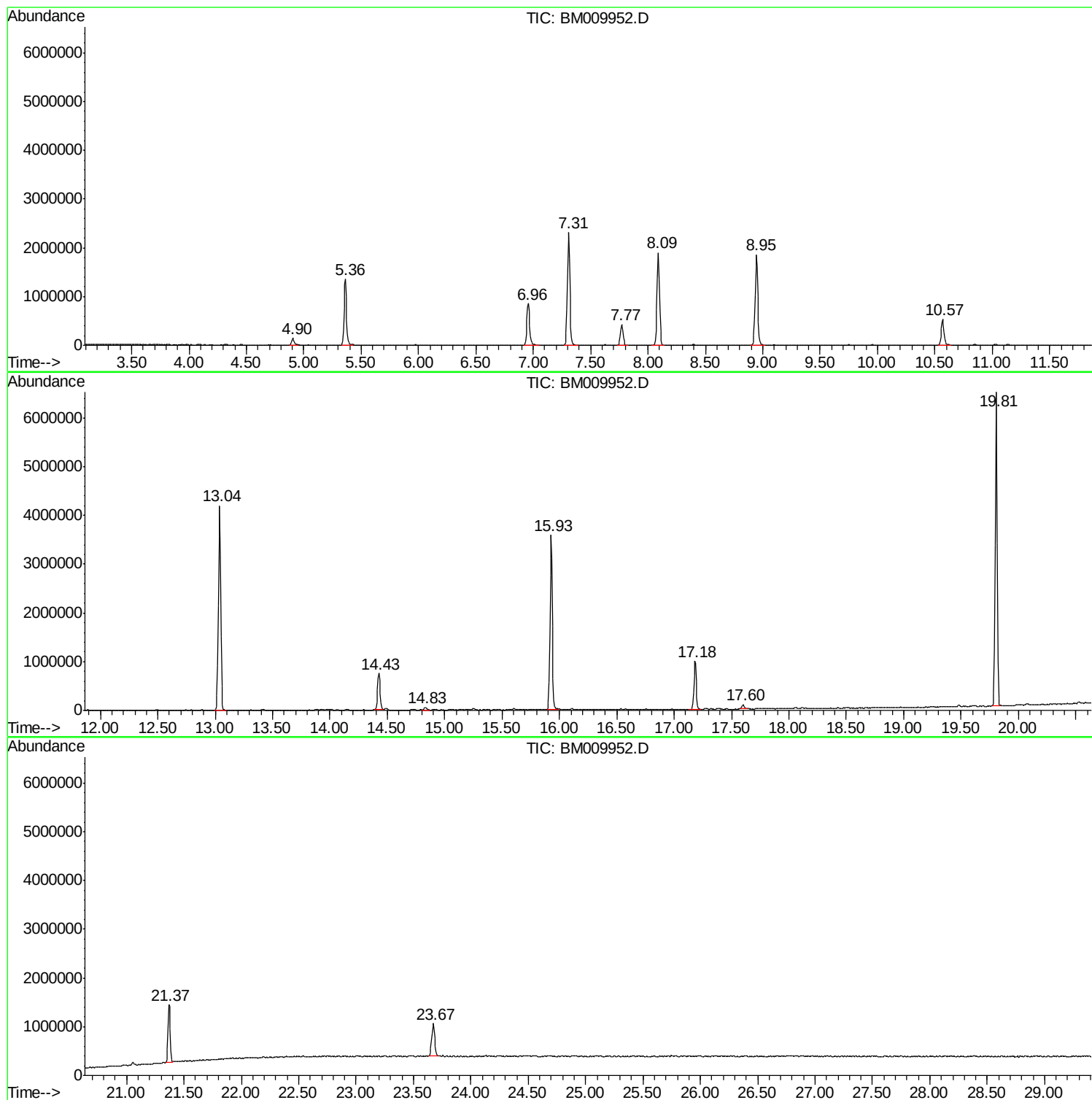
Sum of corrected areas: 39191567

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Quant Method : Z:\HPCHEM1\BNA\_M\METHODS\8270-BM050517.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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Sample : I2992-01  
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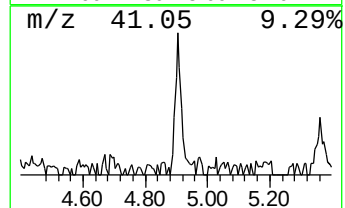
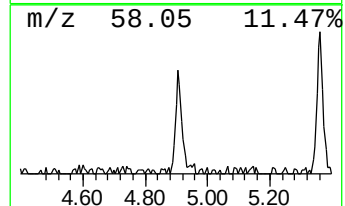
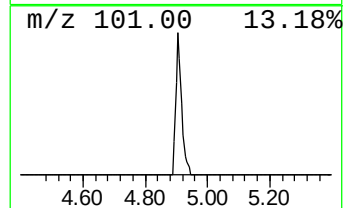
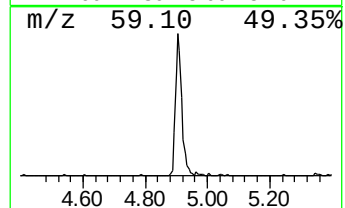
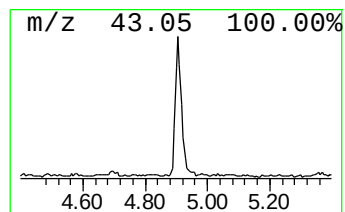
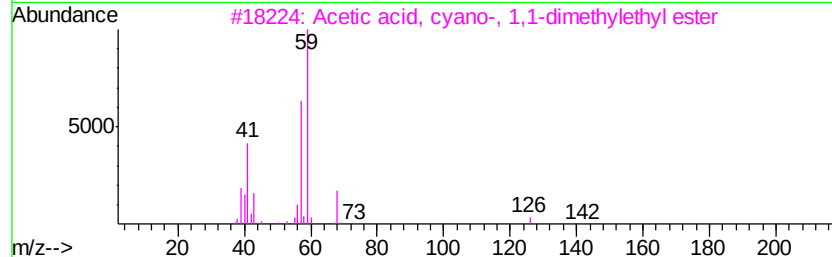
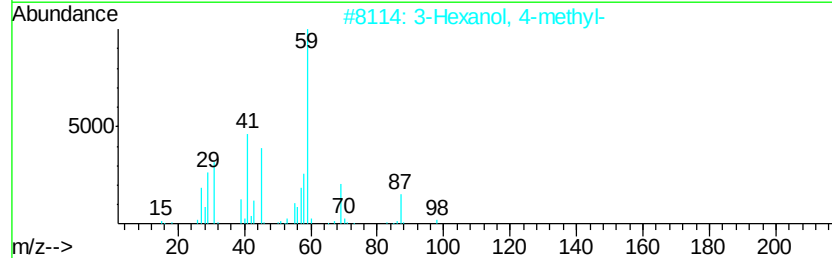
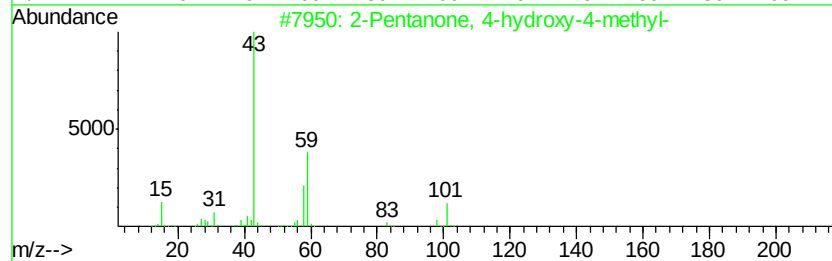
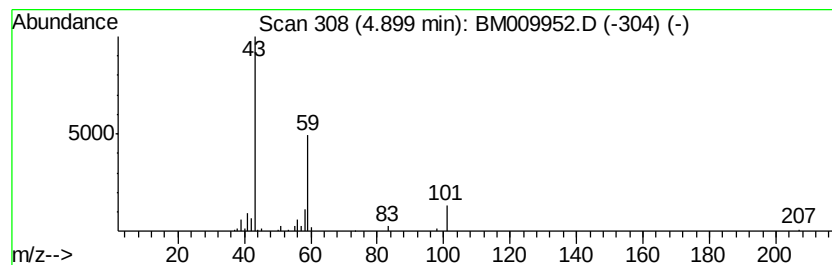
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TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 4.90 | 5.58 ng | 194595 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# of | 5                                   | Tentative ID | MW       | MolForm | CAS#        | Qual |
|---------|-------------------------------------|--------------|----------|---------|-------------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2  |         | 000123-42-2 | 64   |
| 2       | 3-Hexanol, 4-methyl-                | 116          | C7H16O   |         | 000615-29-2 | 33   |
| 3       | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2 |         | 001116-98-9 | 25   |
| 4       | 3-Hydroxy-3-methyl-2-butanone       | 102          | C5H10O2  |         | 000115-22-0 | 23   |
| 5       | Amylene Hydrate                     | 88           | C5H12O   |         | 000075-85-4 | 9    |



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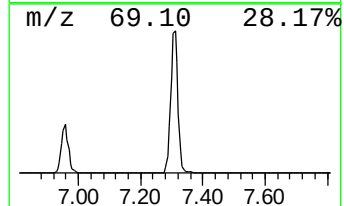
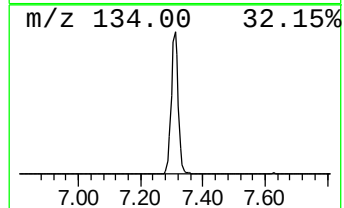
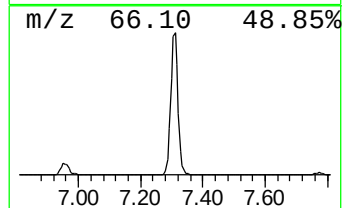
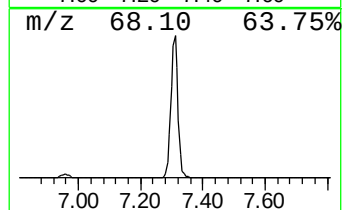
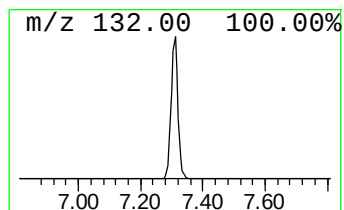
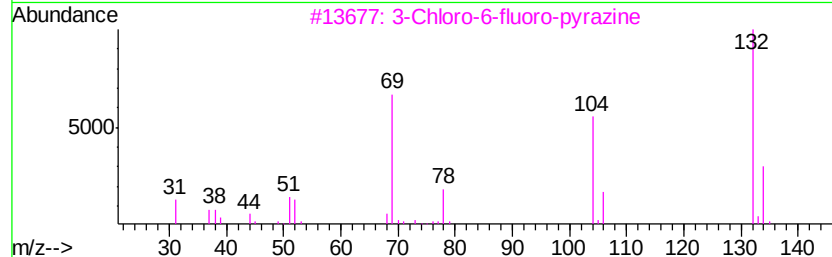
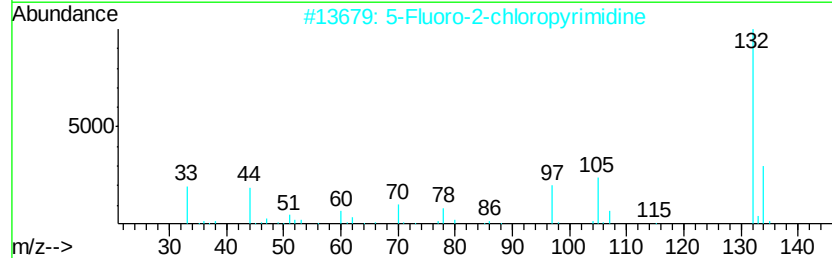
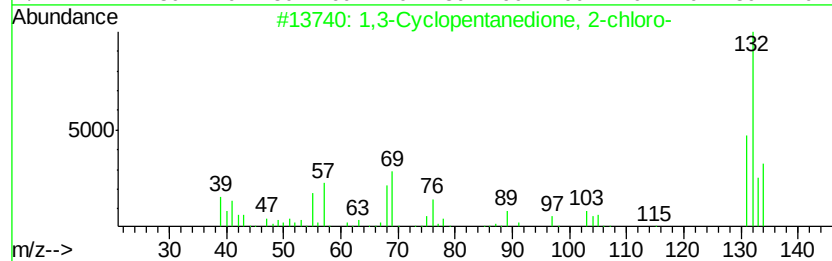
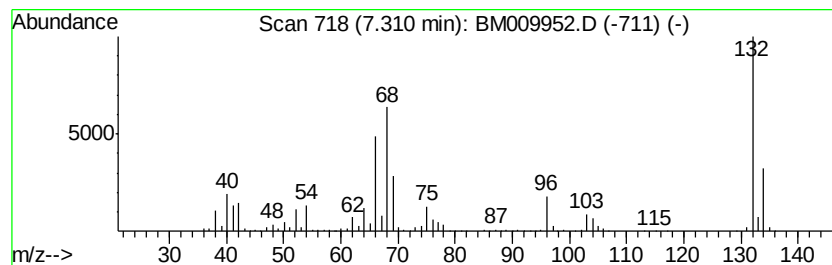
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Peak Number 2 unknown7.31 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.31 | 105.21 ng | 3668940 | 1,4-Dichlorobenzene-d4 | 7.77 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 1,3-Cyclopentanedione, 2-chloro-    | 132 | C5H5ClO2  | 014203-19-1  | 16   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 14   |
| 3    |    | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 4    |    | 3H-1,2-Dithiol-3-one, 5-methyl-     | 132 | C4H4OS2   | 003620-08-4  | 14   |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 10   |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.90 | 5.6     | ng    | 194595   | 1                     | 7.77 | 697474 | 20.0 |
| unknown7.31          | 7.31 | 105.2   | ng    | 3668940  | 1                     | 7.77 | 697474 | 20.0 |