

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090618\  
 Data File : BG036573.D  
 Acq On : 6 Sep 2018 17:30  
 Operator : JU/SJ  
 Sample : J4793-01  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 JCSA-303

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:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG082318.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         | 5.162       | 310           | 319         | 327          | rVB      | 111524         | 179468        | 4.28%           | 0.892%        |
| 2         | 5.626       | 391           | 398         | 409          | rBV      | 841573         | 1328608       | 31.72%          | 6.604%        |
| 3         | 7.212       | 660           | 668         | 685          | rBV      | 756983         | 1294427       | 30.90%          | 6.434%        |
| 4         | 7.588       | 724           | 732         | 746          | rBV      | 904167         | 1540824       | 36.78%          | 7.659%        |
| 5         | 8.058       | 804           | 812         | 819          | rBV      | 202744         | 338076        | 8.07%           | 1.680%        |
| 6         | 8.382       | 859           | 867         | 874          | rBV      | 693313         | 1206779       | 28.81%          | 5.998%        |
| 7         | 9.216       | 1002          | 1009        | 1020         | rVB      | 602091         | 1051280       | 25.10%          | 5.225%        |
| 8         | 10.861      | 1280          | 1289        | 1294         | rBV      | 280313         | 507890        | 12.12%          | 2.525%        |
| 9         | 10.914      | 1294          | 1298        | 1306         | rVB      | 113650         | 192397        | 4.59%           | 0.956%        |
| 10        | 13.305      | 1698          | 1705        | 1714         | rBV      | 1656541        | 2540576       | 60.65%          | 12.628%       |
| 11        | 14.680      | 1933          | 1939        | 1946         | rVB3     | 460585         | 735264        | 17.55%          | 3.655%        |
| 12        | 16.167      | 2185          | 2192        | 2212         | rBV      | 1208758        | 1897243       | 45.29%          | 9.430%        |
| 13        | 17.424      | 2398          | 2406        | 2412         | rBV      | 636958         | 981012        | 23.42%          | 4.876%        |
| 14        | 20.033      | 2843          | 2850        | 2862         | rBV      | 3107568        | 4189049       | 100.00%         | 20.822%       |
| 15        | 21.689      | 3125          | 3132        | 3143         | rBV      | 663355         | 1135054       | 27.10%          | 5.642%        |
| 16        | 24.897      | 3668          | 3678        | 3696         | rBV3     | 316266         | 1000412       | 23.88%          | 4.973%        |

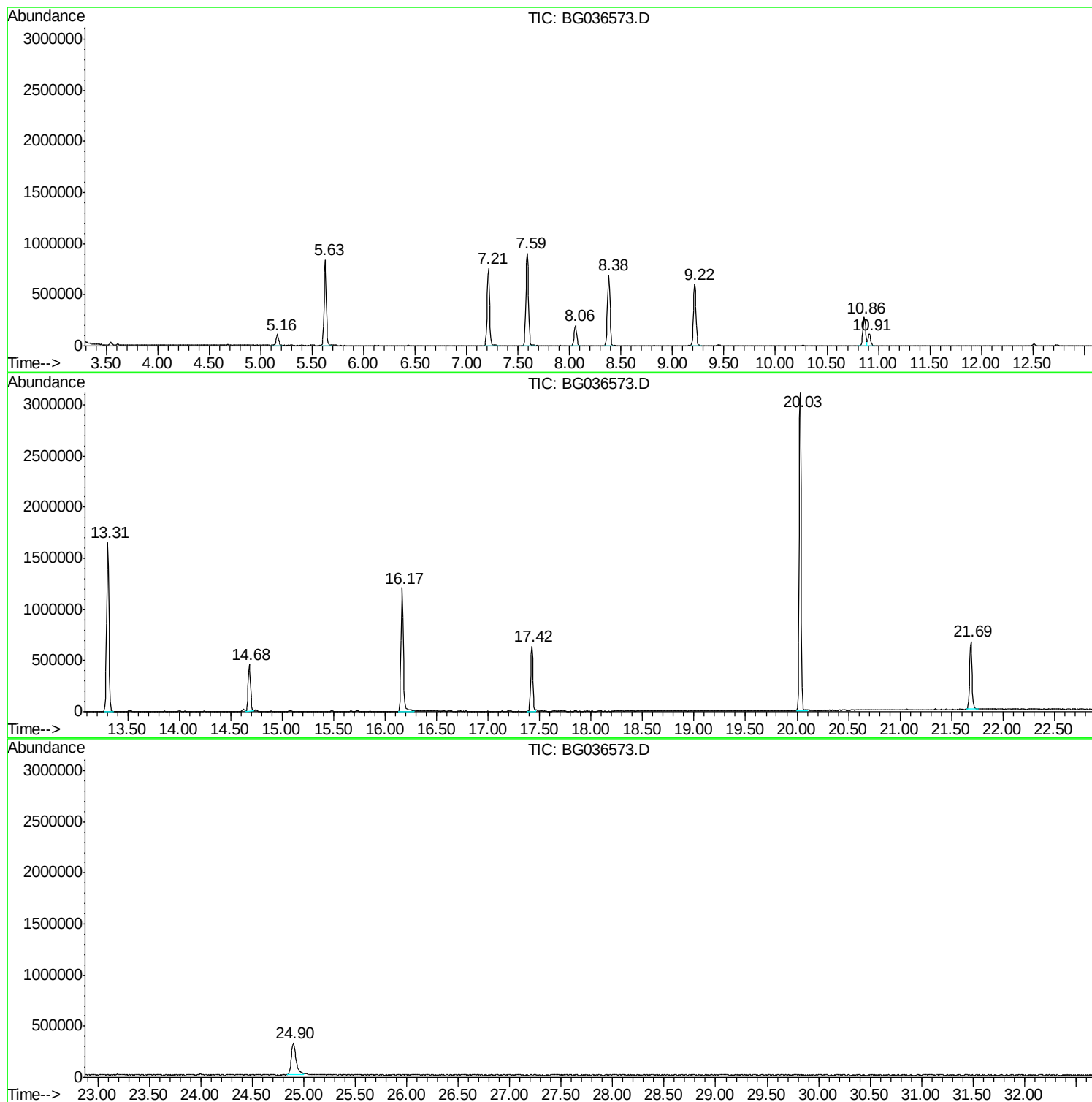
Sum of corrected areas: 20118359

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090618\  
Data File : BG036573.D  
Acq On : 6 Sep 2018 17:30  
Operator : JU/SJ  
Sample : J4793-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
JCSA-303

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090618\  
Data File : BG036573.D  
Acq On : 6 Sep 2018 17:30  
Operator : JU/SJ  
Sample : J4793-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
JCSA-303

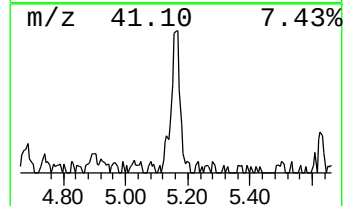
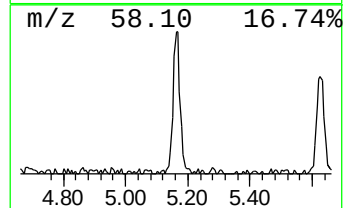
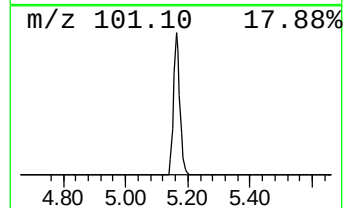
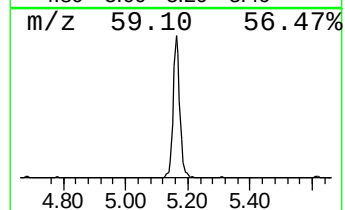
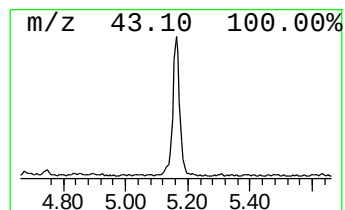
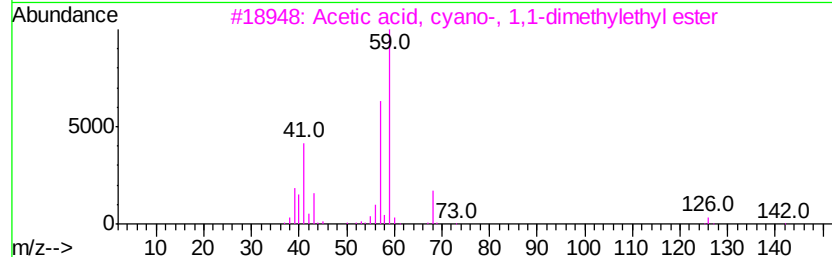
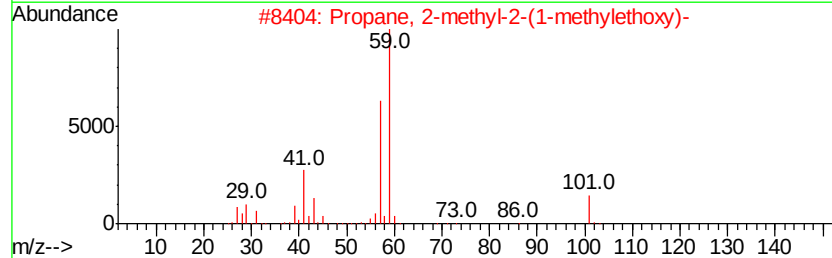
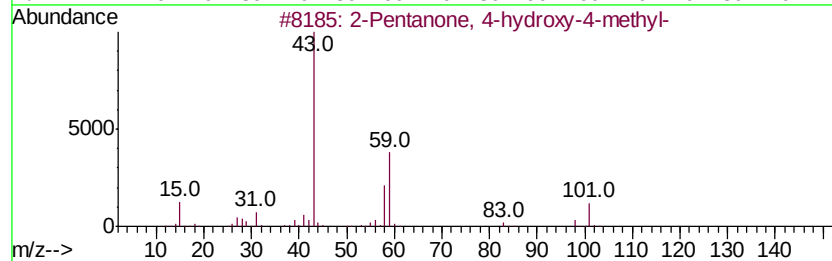
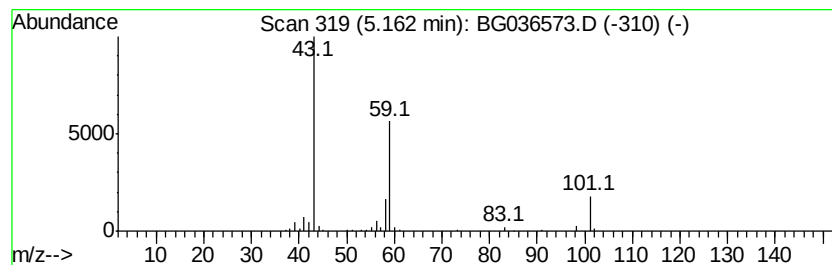
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.16 | 10.62 ng | 179468 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 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    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    |   | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 12   |
| 5    |    |   | 1-Propen-2-ol, acetate               | 100 | C5H8O2   | 000108-22-5 | 10   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090618\  
Data File : BG036573.D  
Acq On : 6 Sep 2018 17:30  
Operator : JU/SJ  
Sample : J4793-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
JCSA-303

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

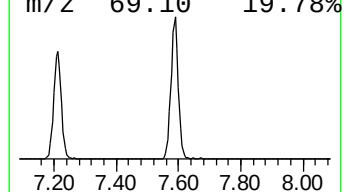
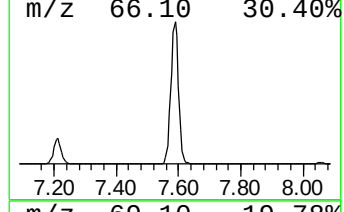
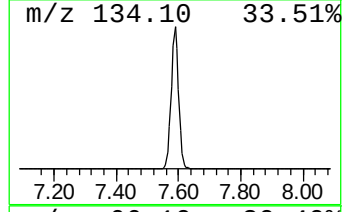
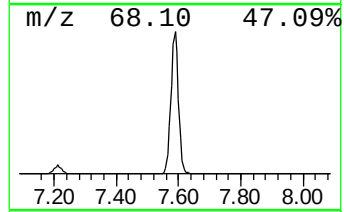
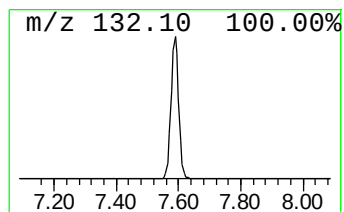
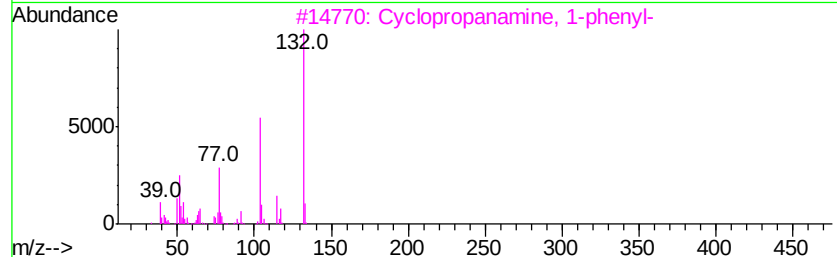
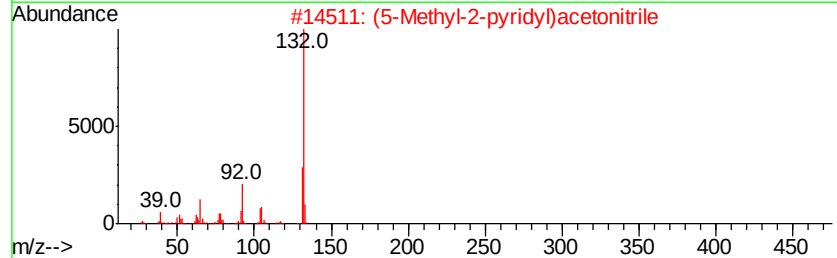
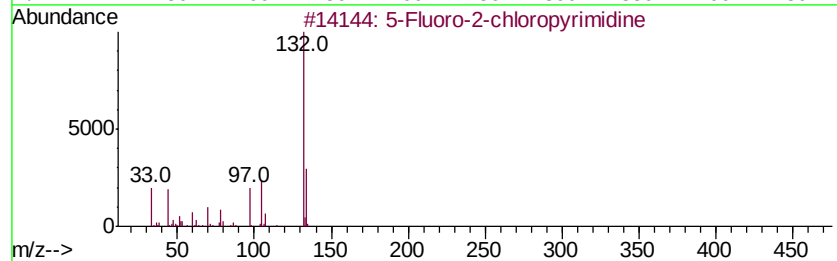
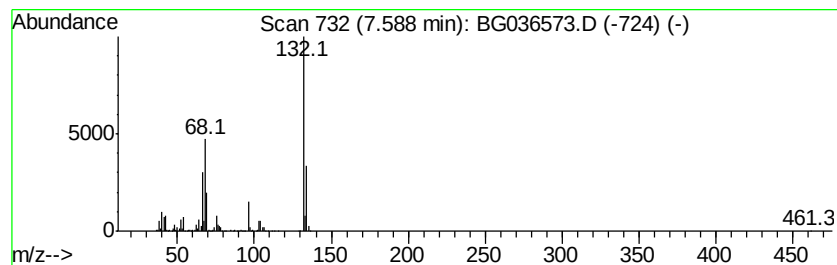
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown7.59 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.59 | 91.15 ng | 1540820 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 2    |    | (5-Methyl-2-pyridyl)acetonitrile    | 132 | C8H8N2    | 1000241-93-9 | 10   |
| 3    |    | Cyclopropanamine, 1-phenyl-         | 133 | C9H11N    | 1000351-26-2 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | Xenon                               | 132 | Xe        | 007440-63-3  | 9    |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_G\DATA\BG090618\  
Data File : BG036573.D  
Acq On : 6 Sep 2018 17:30  
Operator : JU/SJ  
Sample : J4793-01  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
JCSA-303

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG082318.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.16 | 10.6    | ng    | 179468   | 1                     | 8.06 | 338076 | 20.0 |
| unknown7.59          | 7.59 | 91.2    | ng    | 1540820  | 1                     | 8.06 | 338076 | 20.0 |