

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG090618\  
 Data File : BG036592.D  
 Acq On : 7 Sep 2018 11:50  
 Operator : JU/SJ  
 Sample : PB112623BL  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB112623BL

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         | 5.159       | 312           | 318         | 325          | rBV      | 40047          | 59612         | 1.39%           | 0.286%        |
| 2         | 5.623       | 390           | 397         | 410          | rBV      | 989896         | 1541094       | 35.83%          | 7.390%        |
| 3         | 7.210       | 659           | 667         | 677          | rBV      | 1020888        | 1725570       | 40.11%          | 8.275%        |
| 4         | 7.586       | 722           | 731         | 744          | rBV      | 944362         | 1592098       | 37.01%          | 7.635%        |
| 5         | 8.056       | 803           | 811         | 819          | rVB      | 197023         | 320376        | 7.45%           | 1.536%        |
| 6         | 8.379       | 858           | 866         | 875          | rBV      | 671400         | 1163810       | 27.05%          | 5.581%        |
| 7         | 9.213       | 1000          | 1008        | 1020         | rBV      | 584151         | 1036514       | 24.10%          | 4.970%        |
| 8         | 10.858      | 1281          | 1288        | 1298         | rVB      | 265540         | 480339        | 11.17%          | 2.303%        |
| 9         | 13.303      | 1697          | 1704        | 1716         | rBV      | 1715121        | 2606966       | 60.60%          | 12.501%       |
| 10        | 14.677      | 1932          | 1938        | 1948         | rVB2     | 468125         | 749993        | 17.43%          | 3.596%        |
| 11        | 16.164      | 2184          | 2191        | 2212         | rBV      | 1259491        | 1938317       | 45.06%          | 9.295%        |
| 12        | 17.421      | 2398          | 2405        | 2413         | rBV2     | 660062         | 1001395       | 23.28%          | 4.802%        |
| 13        | 19.724      | 2793          | 2797        | 2802         | rBV      | 54331          | 59056         | 1.37%           | 0.283%        |
| 14        | 20.030      | 2842          | 2849        | 2860         | rBV      | 3316258        | 4301672       | 100.00%         | 20.628%       |
| 15        | 20.764      | 2970          | 2974        | 2982         | rVB      | 44308          | 51446         | 1.20%           | 0.247%        |
| 16        | 21.687      | 3124          | 3131        | 3146         | rBV      | 698460         | 1161959       | 27.01%          | 5.572%        |
| 17        | 24.895      | 3666          | 3677        | 3703         | rBV      | 312657         | 1063772       | 24.73%          | 5.101%        |

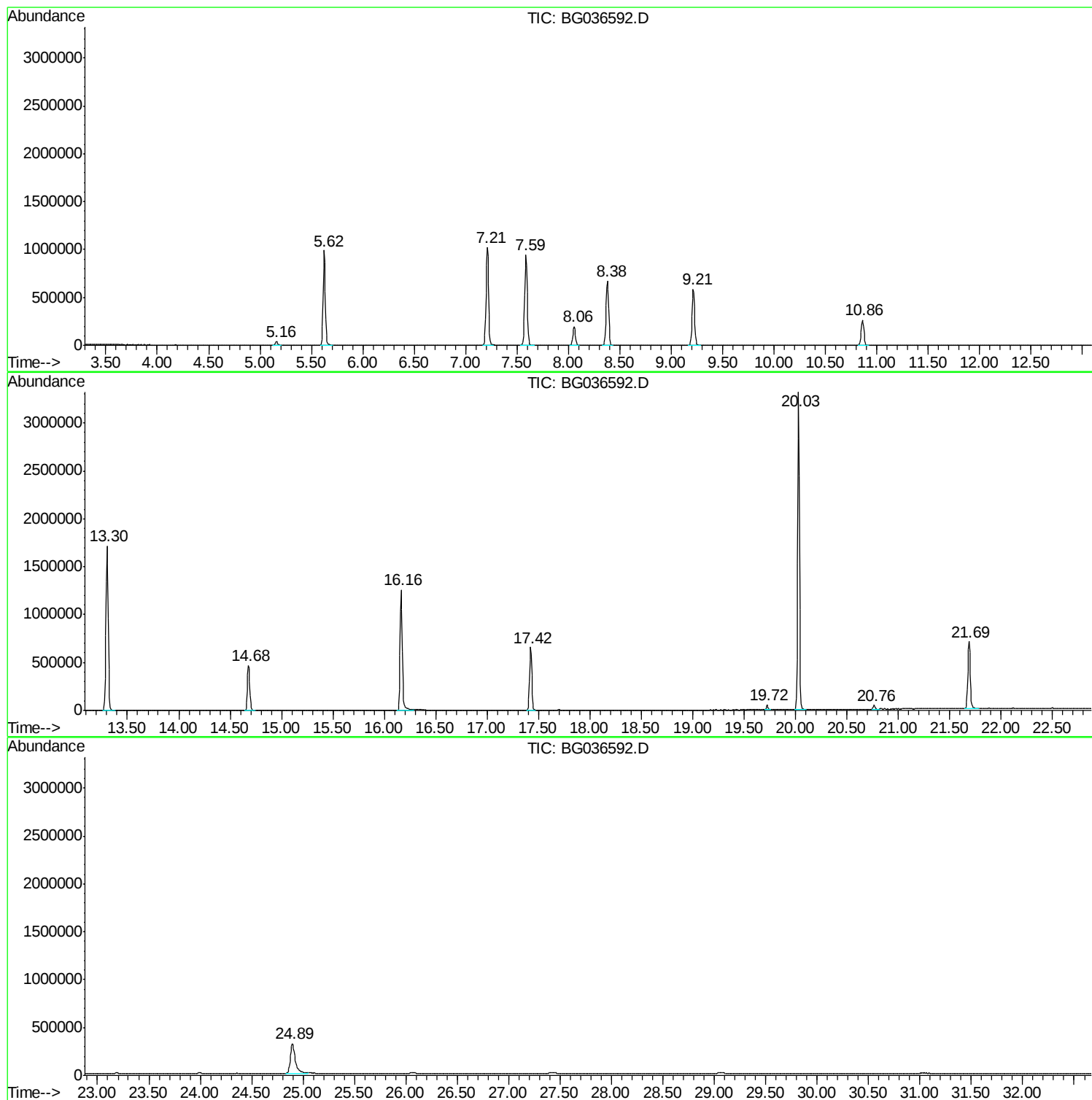
Sum of corrected areas: 20853989

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



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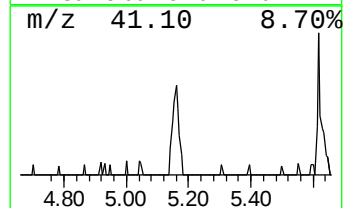
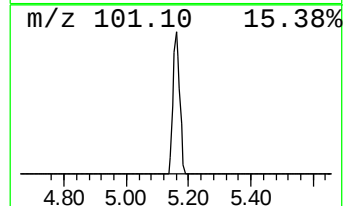
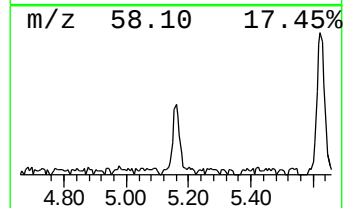
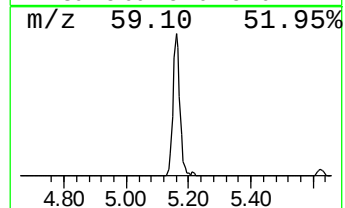
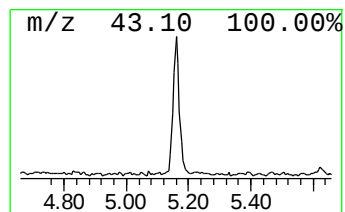
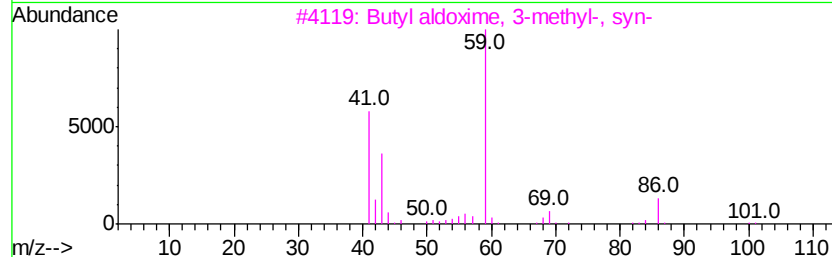
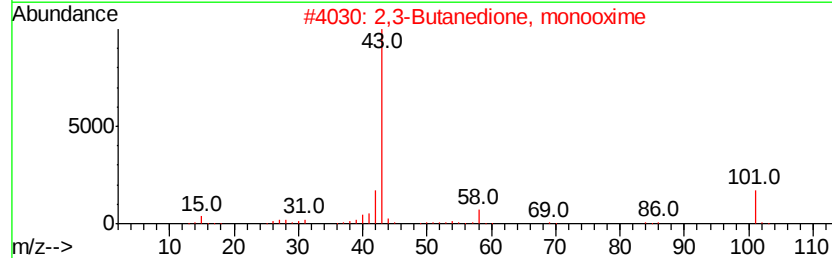
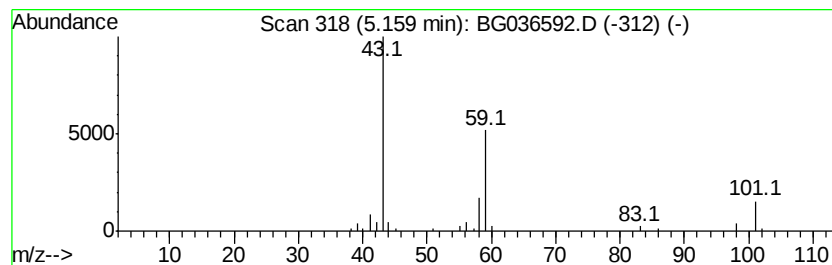
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.16 | 3.72 ng | 59612 | 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 | 56   |
| 2    |    |   | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 35   |
| 3    |    |   | Butyl aldoxime, 3-methyl-, syn-  | 101 | C5H11NO | 005780-40-5 | 23   |
| 4    |    |   | 5-Hexen-2-one                    | 98  | C6H10O  | 000109-49-9 | 9    |
| 5    |    |   | Morpholine, 4-methyl-            | 101 | C5H11NO | 000109-02-4 | 9    |



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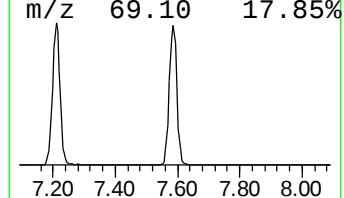
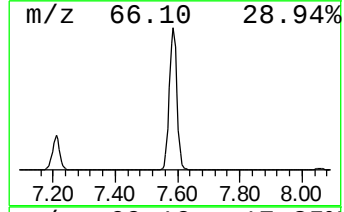
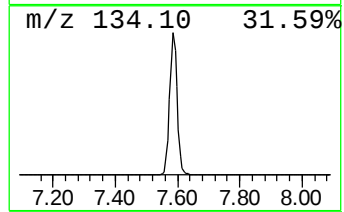
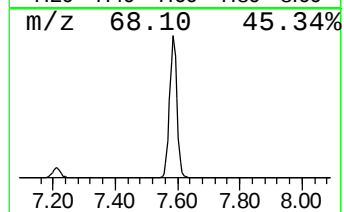
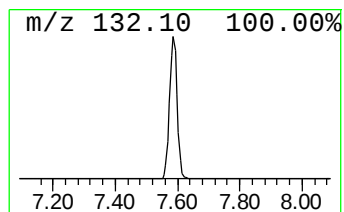
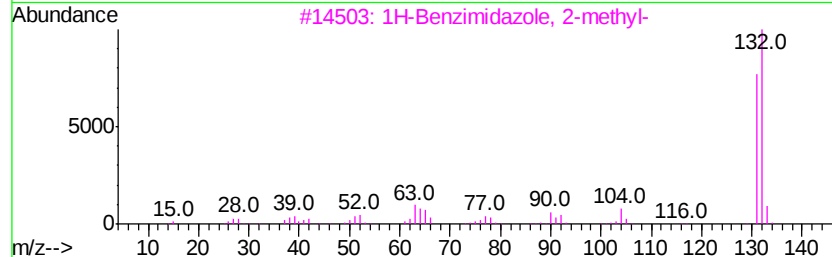
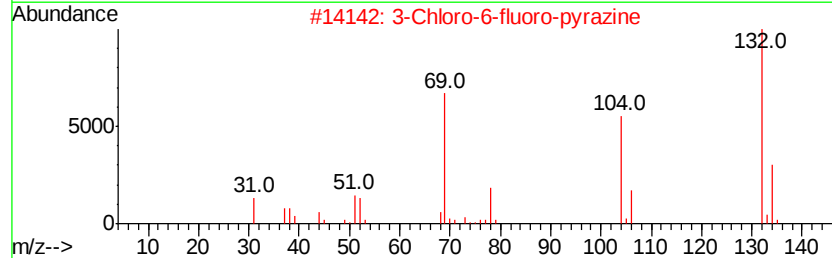
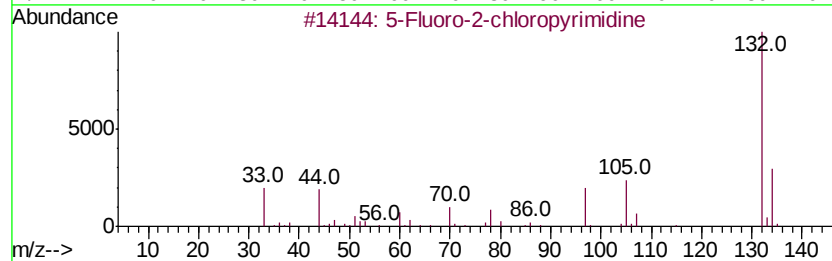
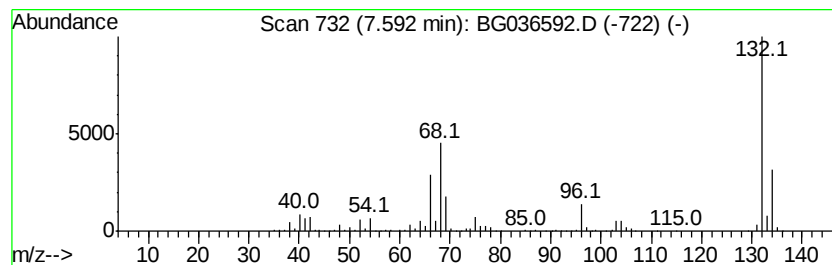
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Peak Number 2 unknown7.59 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.59 | 99.39 ng | 1592100 | 1,4-Dichlorobenzene-d4 | 8.06 |

| Hit# | of                                  | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-----------|--------------|------|------|
| 1    | 5-Fluoro-2-chloropyrimidine         | 132          | C4H2ClFN2 | 062802-42-0  | 27   |      |
| 2    | 3-Chloro-6-fluoro-pyrazine          | 132          | C4H2ClFN2 | 1000146-10-7 | 27   |      |
| 3    | 1H-Benzimidazole, 2-methyl-         | 132          | C8H8N2    | 000615-15-6  | 22   |      |
| 4    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132          | C10H12    | 028749-81-7  | 9    |      |
| 5    | 4-Chloro-2-fluoropyrimidine         | 132          | C4H2ClFN2 | 051422-00-5  | 9    |      |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 5.16 | 3.7     | ng    | 59612    | 1                     | 8.06 | 320376 | 20.0 |
| unknown7.59          | 7.59 | 99.4    | ng    | 1592100  | 1                     | 8.06 | 320376 | 20.0 |