

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081016\  
 Data File : BF089702.D  
 Acq On : 10 Aug 2016 18:36  
 Operator : UM/SJ  
 Sample : PB92598BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB92598BL

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-BF080416.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         | 4.616       | 262           | 265         | 284          | rBV      | 161186         | 389591        | 23.73%          | 3.096%        |
| 2         | 5.302       | 323           | 325         | 345          | rBV      | 638348         | 1214157       | 73.95%          | 9.649%        |
| 3         | 6.947       | 466           | 469         | 476          | rBV      | 677816         | 1180031       | 71.87%          | 9.377%        |
| 4         | 7.050       | 476           | 478         | 495          | rVB      | 955268         | 1442754       | 87.87%          | 11.465%       |
| 5         | 7.393       | 507           | 508         | 526          | rVB      | 133990         | 288687        | 17.58%          | 2.294%        |
| 6         | 7.633       | 526           | 529         | 543          | rBV      | 756658         | 1051944       | 64.07%          | 8.359%        |
| 7         | 8.308       | 586           | 588         | 611          | rBV      | 479503         | 806798        | 49.14%          | 6.411%        |
| 8         | 9.428       | 683           | 686         | 704          | rBV      | 251490         | 403377        | 24.57%          | 3.206%        |
| 9         | 11.211      | 838           | 842         | 862          | rBV      | 1148049        | 1641876       | 100.00%         | 13.047%       |
| 10        | 12.251      | 930           | 933         | 944          | rBB      | 340959         | 481343        | 29.32%          | 3.825%        |
| 11        | 13.542      | 1043          | 1046        | 1057         | rBV      | 613870         | 874299        | 53.25%          | 6.948%        |
| 12        | 14.640      | 1140          | 1142        | 1153         | rBV      | 330694         | 485038        | 29.54%          | 3.854%        |
| 13        | 17.017      | 1347          | 1350        | 1353         | rBV      | 1107949        | 1597357       | 97.29%          | 12.694%       |
| 14        | 18.354      | 1465          | 1467        | 1478         | rBV      | 327340         | 411894        | 25.09%          | 3.273%        |
| 15        | 20.012      | 1610          | 1612        | 1621         | rBV      | 181887         | 314715        | 19.17%          | 2.501%        |

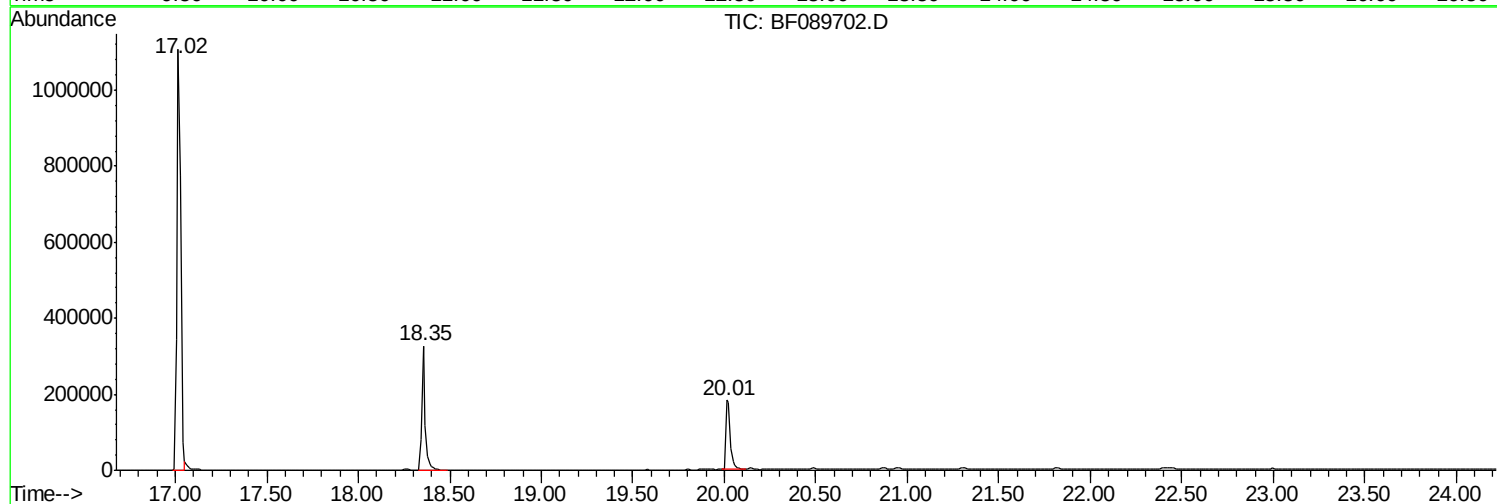
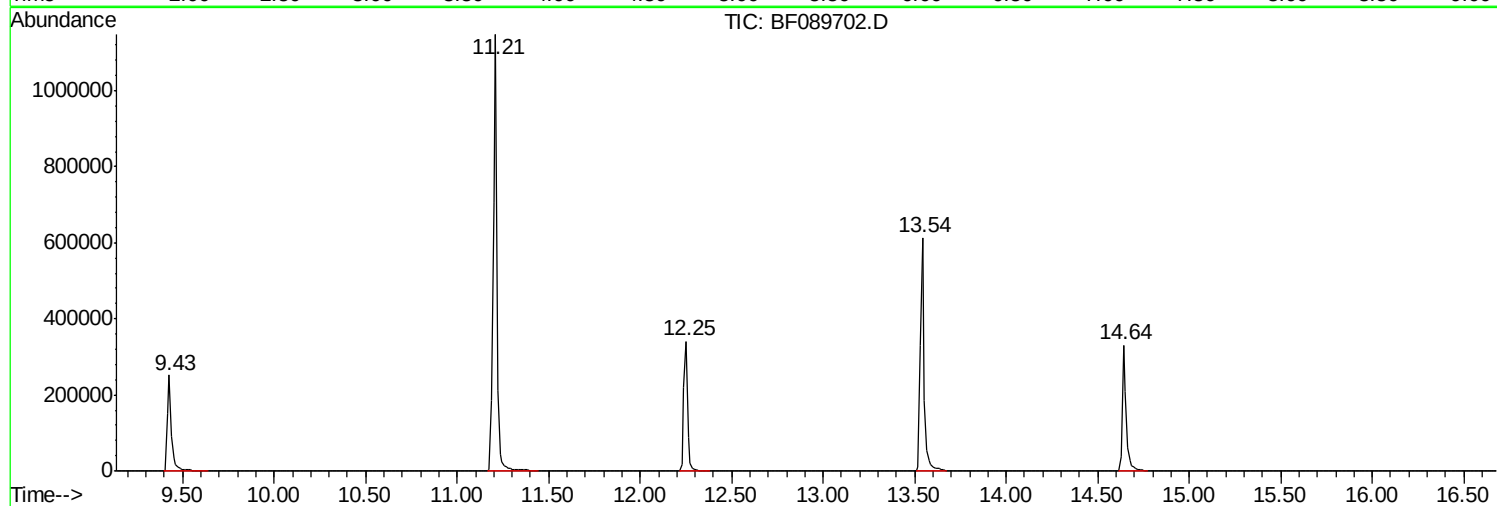
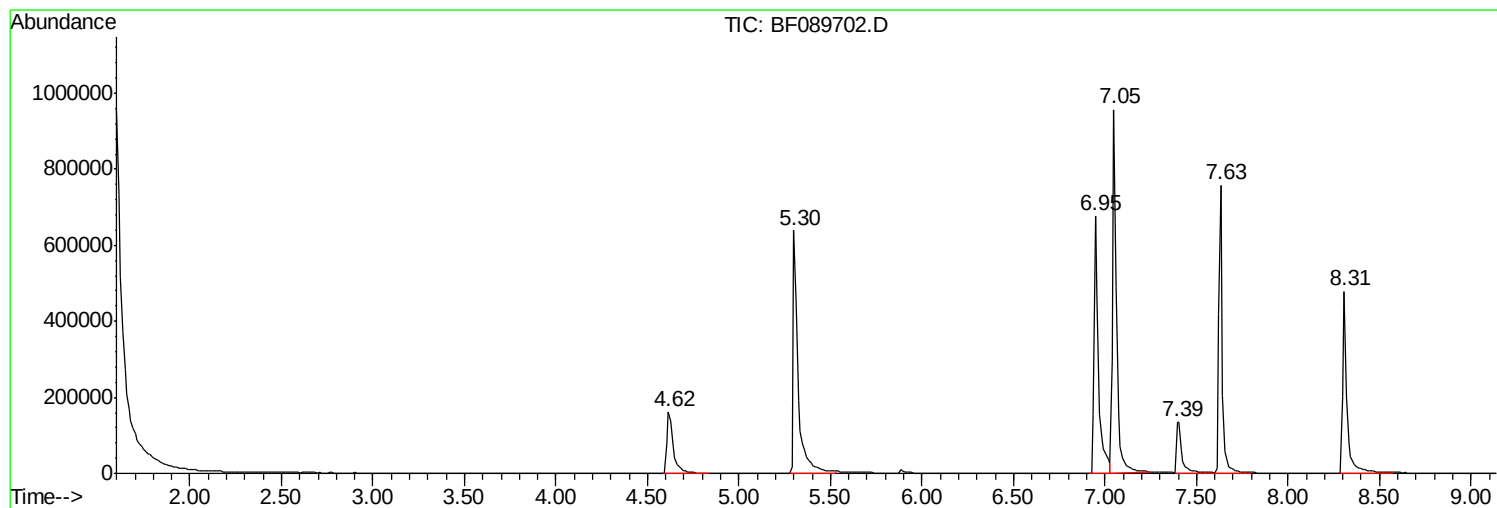
Sum of corrected areas: 12583861

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



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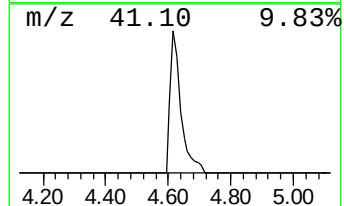
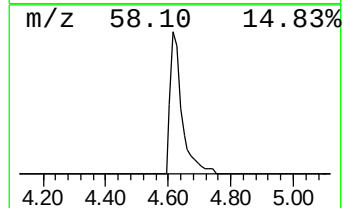
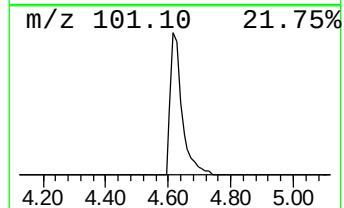
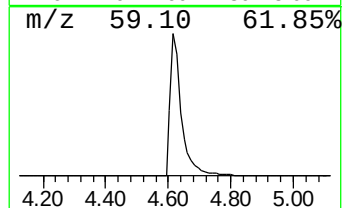
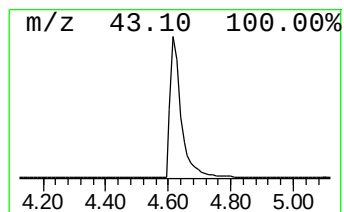
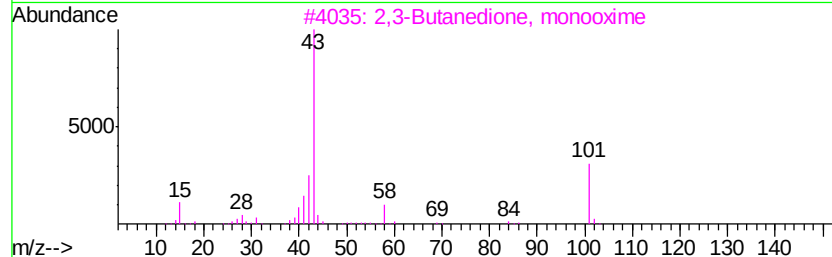
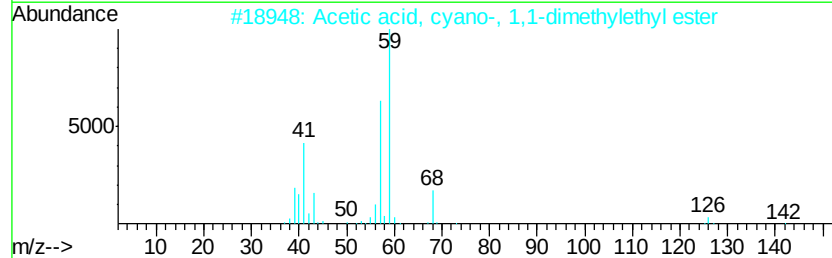
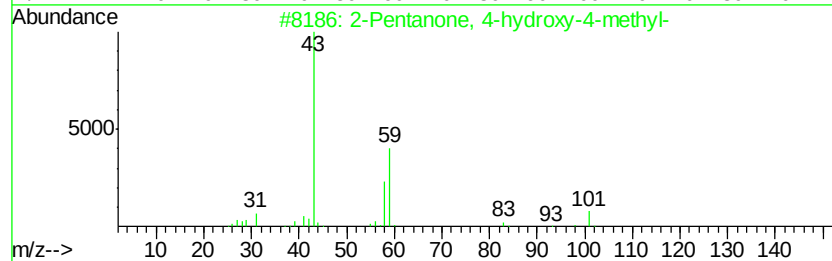
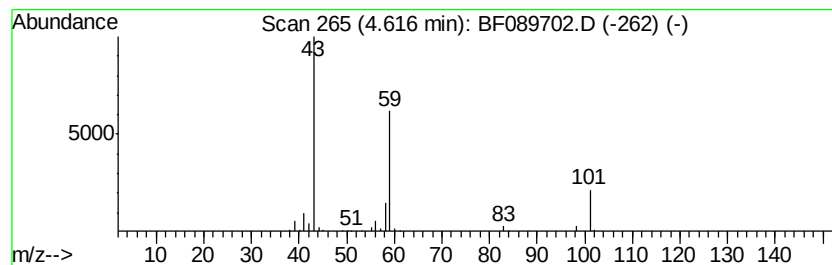
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.62 | 26.99 ng | 389591 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 17   |
| 4    |    | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |
| 5    |    | 3-Pentanol, 2-methyl-               | 102 | C6H14O   | 000565-67-3 | 9    |



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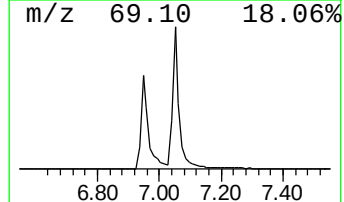
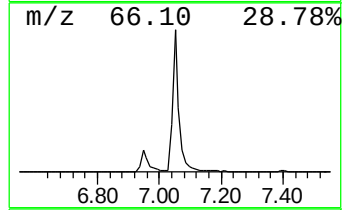
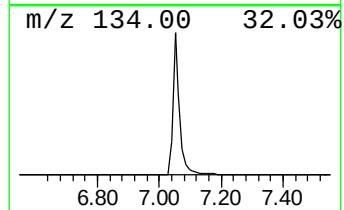
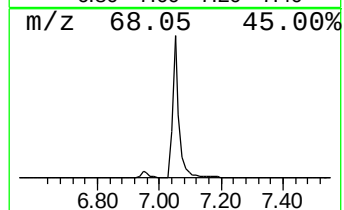
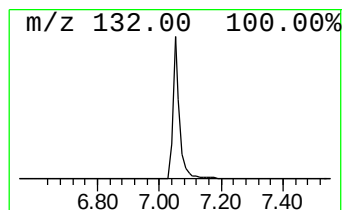
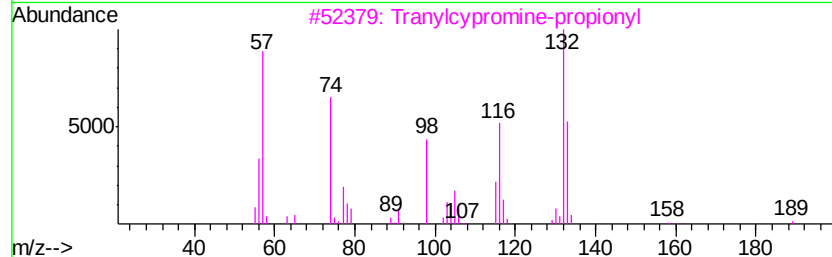
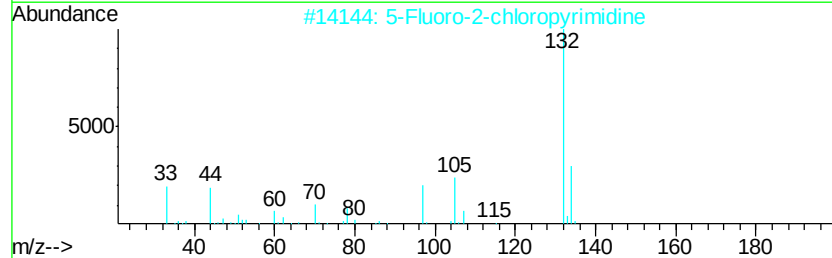
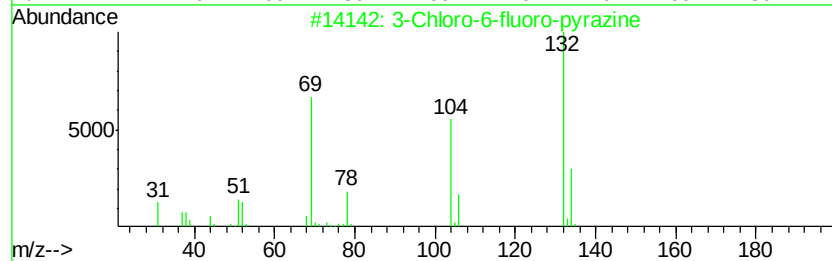
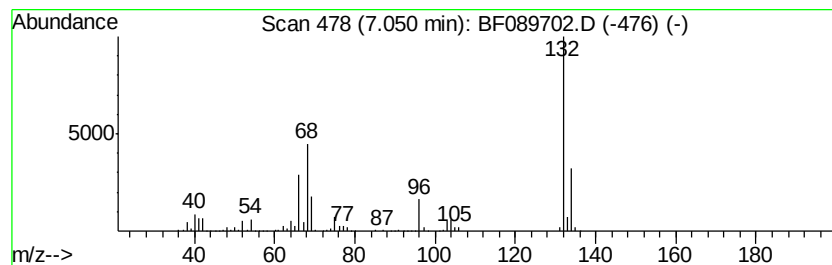
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Peak Number 2 unknown7.05 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.05 | 99.95 ng | 1442750 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# | of | Tentative ID                   | MW  | MolForm   | CAS#         | Qual |
|------|----|--------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine     | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | 5-Fluoro-2-chloropyrimidine    | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 3    |    | Tranylcypromine-propionyl      | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine   | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2    | 064608-59-9  | 9    |



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| TIC Top Hit name     | RT   | EstConc | Units | Response | --Internal Standard-- |      |        |      |
|----------------------|------|---------|-------|----------|-----------------------|------|--------|------|
|                      |      |         |       |          | #                     | RT   | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.62 | 27.0    | ng    | 389591   | 1                     | 7.40 | 288687 | 20.0 |
| unknown7.05          | 7.05 | 100.0   | ng    | 1442750  | 1                     | 7.40 | 288687 | 20.0 |