

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF061518\  
 Data File : BF106498.D  
 Acq On : 15 Jun 2018 18:07  
 Operator : JU/SJ  
 Sample : J3504-01  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-44COMP

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0

Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061118.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         | 5.201       | 483           | 487         | 494          | rVB      | 203003         | 229502        | 9.98%           | 1.081%        |
| 2         | 5.607       | 553           | 556         | 563          | rBV      | 2130712        | 2255963       | 98.11%          | 10.628%       |
| 3         | 6.607       | 722           | 726         | 739          | rBV      | 2437098        | 2246723       | 97.71%          | 10.584%       |
| 4         | 6.742       | 745           | 749         | 753          | rBV      | 2471167        | 2226753       | 96.84%          | 10.490%       |
| 5         | 6.966       | 783           | 787         | 790          | rBV      | 968659         | 766327        | 33.33%          | 3.610%        |
| 6         | 7.119       | 809           | 813         | 817          | rBV      | 1847862        | 1728768       | 75.19%          | 8.144%        |
| 7         | 7.525       | 877           | 882         | 885          | rBV      | 1525693        | 1482070       | 64.46%          | 6.982%        |
| 8         | 8.248       | 1001          | 1005        | 1008         | rBV      | 1107461        | 931878        | 40.53%          | 4.390%        |
| 9         | 9.319       | 1183          | 1187        | 1191         | rBV      | 2494686        | 2299336       | 100.00%         | 10.832%       |
| 10        | 9.713       | 1250          | 1254        | 1262         | rVB      | 266319         | 231753        | 10.08%          | 1.092%        |
| 11        | 9.919       | 1285          | 1289        | 1293         | rBV      | 44411          | 35781         | 1.56%           | 0.169%        |
| 12        | 10.007      | 1300          | 1304        | 1308         | rBV      | 1045532        | 915765        | 39.83%          | 4.314%        |
| 13        | 10.419      | 1372          | 1374        | 1377         | rVB      | 59866          | 43017         | 1.87%           | 0.203%        |
| 14        | 10.795      | 1434          | 1438        | 1442         | rBV      | 1268561        | 1213467       | 52.77%          | 5.717%        |
| 15        | 10.895      | 1451          | 1455        | 1460         | rBV      | 43598          | 48150         | 2.09%           | 0.227%        |
| 16        | 11.495      | 1554          | 1557        | 1561         | rBV      | 879561         | 766256        | 33.33%          | 3.610%        |
| 17        | 13.083      | 1823          | 1827        | 1830         | rBV      | 2203516        | 1892174       | 82.29%          | 8.914%        |
| 18        | 13.971      | 1974          | 1978        | 1985         | rVB2     | 66544          | 88081         | 3.83%           | 0.415%        |
| 19        | 14.148      | 2004          | 2008        | 2012         | rBV      | 1026183        | 919473        | 39.99%          | 4.332%        |
| 20        | 14.612      | 2084          | 2087        | 2091         | rBV4     | 26975          | 35800         | 1.56%           | 0.169%        |
| 21        | 15.289      | 2200          | 2202        | 2207         | rVB2     | 21042          | 24193         | 1.05%           | 0.114%        |
| 22        | 15.695      | 2265          | 2271        | 2277         | rBV      | 630445         | 818219        | 35.59%          | 3.855%        |
| 23        | 16.159      | 2348          | 2350        | 2355         | rVB3     | 23629          | 27119         | 1.18%           | 0.128%        |

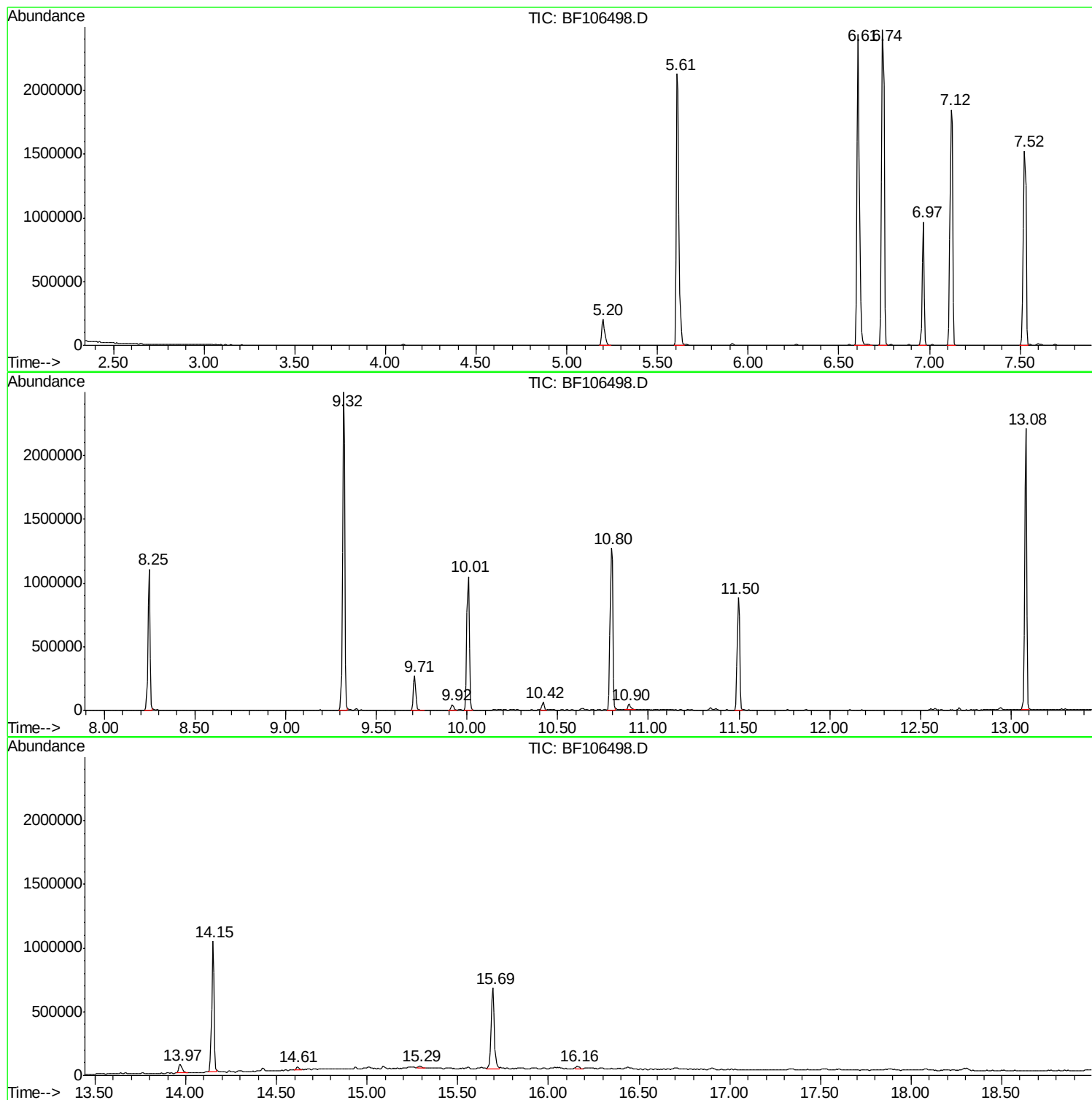
Sum of corrected areas: 21226568

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF061118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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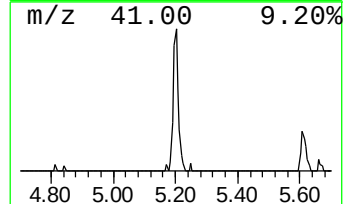
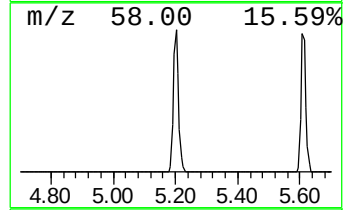
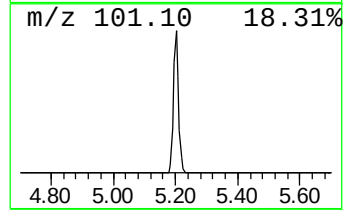
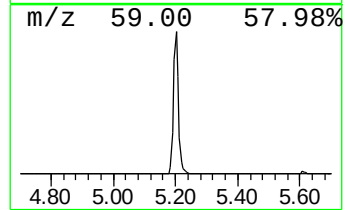
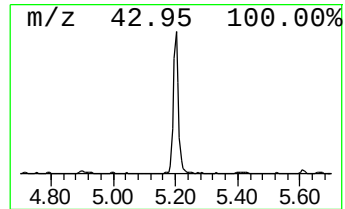
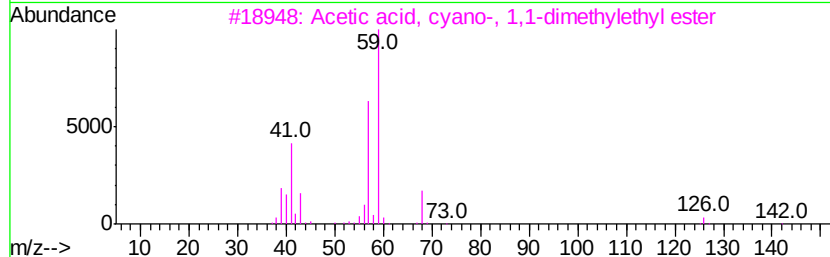
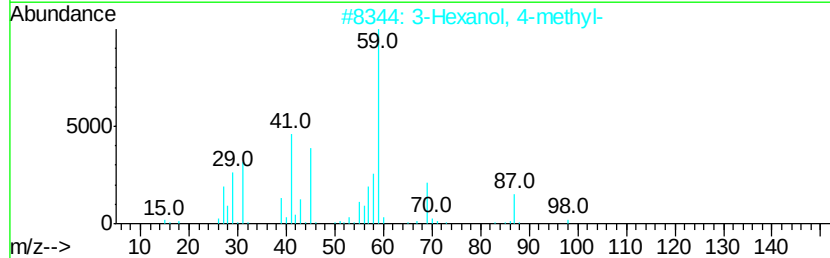
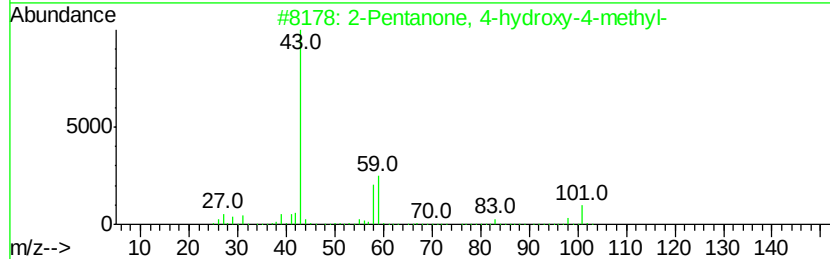
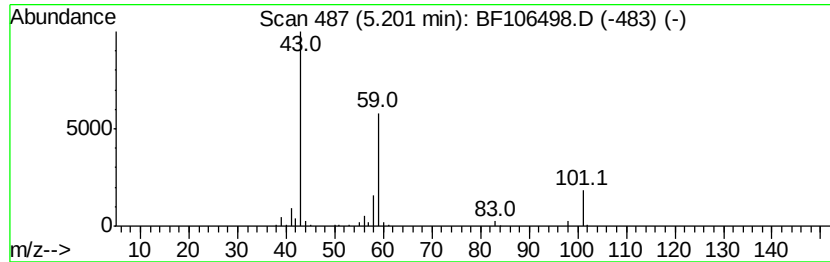
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.20 | 5.99 ng | 229502 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    |   | 3-Hexanol, 4-methyl-                 | 116 | C7H16O   | 000615-29-2 | 33   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    |   | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 10   |
| 5    |    |   | 3-Hexanol, 4-ethyl-                  | 130 | C8H18O   | 019780-44-0 | 9    |



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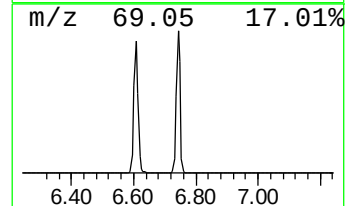
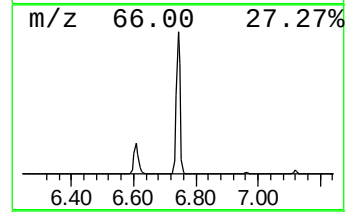
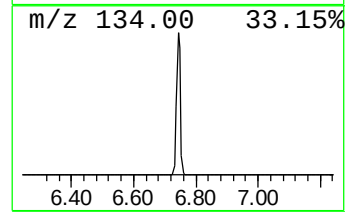
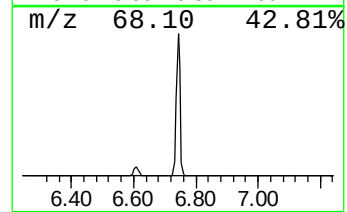
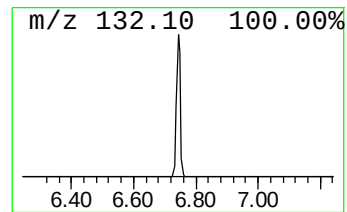
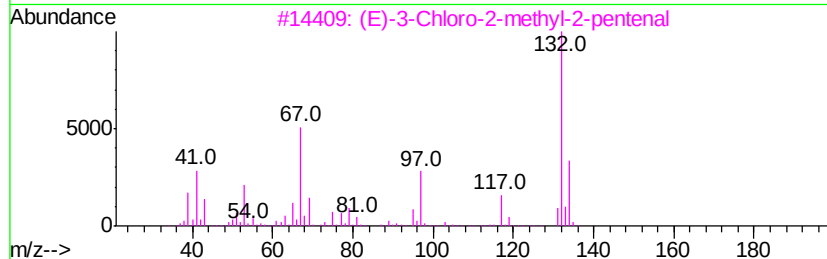
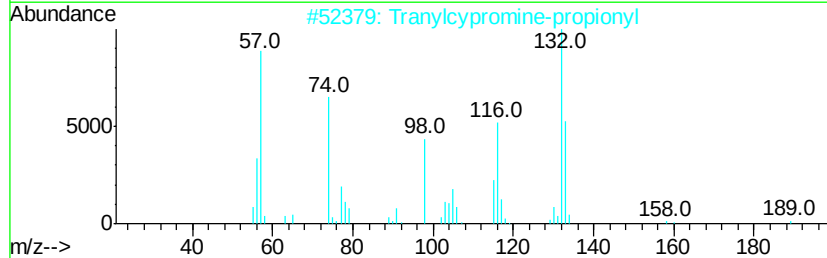
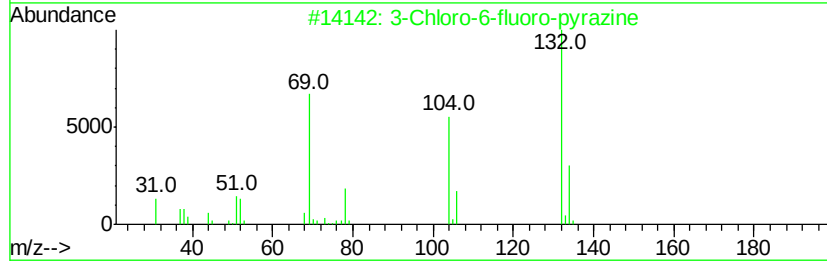
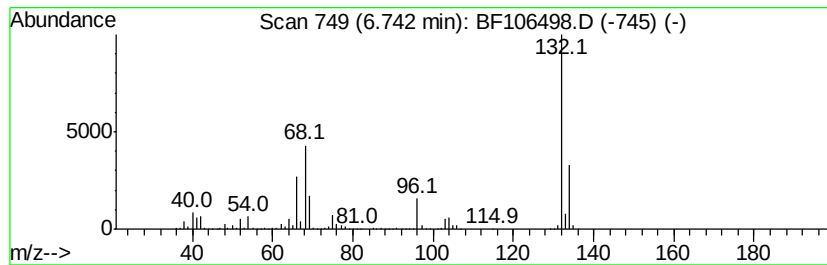
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Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 58.12 ng | 2226750 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 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... | 5.20 | 6.0     | ng    | 229502   | 1                     | 6.97 | 766327 | 20.0 |
| unknown6.74          | 6.74 | 58.1    | ng    | 2226750  | 1                     | 6.97 | 766327 | 20.0 |