

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF031815\  
 Data File : BF077813.D  
 Acq On : 19 Mar 2015 1:25  
 Operator : TP/IZ  
 Sample : PB82167BL  
 Misc :  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB82167BL

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-BF031115.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         | 1.321       | 36            | 38          | 41           | rBV      | 3048982        | 3347535       | 100.00%         | 23.542%       |
| 2         | 1.435       | 45            | 48          | 51           | rVB      | 17875          | 35691         | 1.07%           | 0.251%        |
| 3         | 1.790       | 76            | 79          | 88           | rVB      | 27578          | 42710         | 1.28%           | 0.300%        |
| 4         | 4.921       | 351           | 353         | 361          | rBV      | 112491         | 166312        | 4.97%           | 1.170%        |
| 5         | 5.447       | 396           | 399         | 401          | rBV      | 774417         | 1050937       | 31.39%          | 7.391%        |
| 6         | 6.727       | 508           | 511         | 513          | rBV      | 1149651        | 1100158       | 32.86%          | 7.737%        |
| 7         | 6.865       | 521           | 523         | 526          | rBV      | 1015305        | 1107332       | 33.08%          | 7.787%        |
| 8         | 7.162       | 547           | 549         | 551          | rBV      | 234780         | 238233        | 7.12%           | 1.675%        |
| 9         | 7.345       | 563           | 565         | 567          | rBV      | 983631         | 894823        | 26.73%          | 6.293%        |
| 10        | 7.847       | 607           | 609         | 612          | rBV      | 546064         | 627998        | 18.76%          | 4.416%        |
| 11        | 8.739       | 684           | 687         | 689          | rBV      | 272688         | 313838        | 9.38%           | 2.207%        |
| 12        | 10.076      | 802           | 804         | 807          | rBV      | 1032512        | 1351030       | 40.36%          | 9.501%        |
| 13        | 10.899      | 874           | 876         | 879          | rBV      | 268781         | 357459        | 10.68%          | 2.514%        |
| 14        | 11.882      | 960           | 962         | 965          | rBV      | 773108         | 730599        | 21.82%          | 5.138%        |
| 15        | 12.739      | 1035          | 1037        | 1040         | rBV      | 361109         | 374916        | 11.20%          | 2.637%        |
| 16        | 14.740      | 1209          | 1212        | 1215         | rBV      | 1660016        | 1618380       | 48.35%          | 11.381%       |
| 17        | 16.020      | 1322          | 1324        | 1327         | rBV      | 380673         | 431320        | 12.88%          | 3.033%        |
| 18        | 17.723      | 1471          | 1473        | 1480         | rBV      | 277651         | 430296        | 12.85%          | 3.026%        |

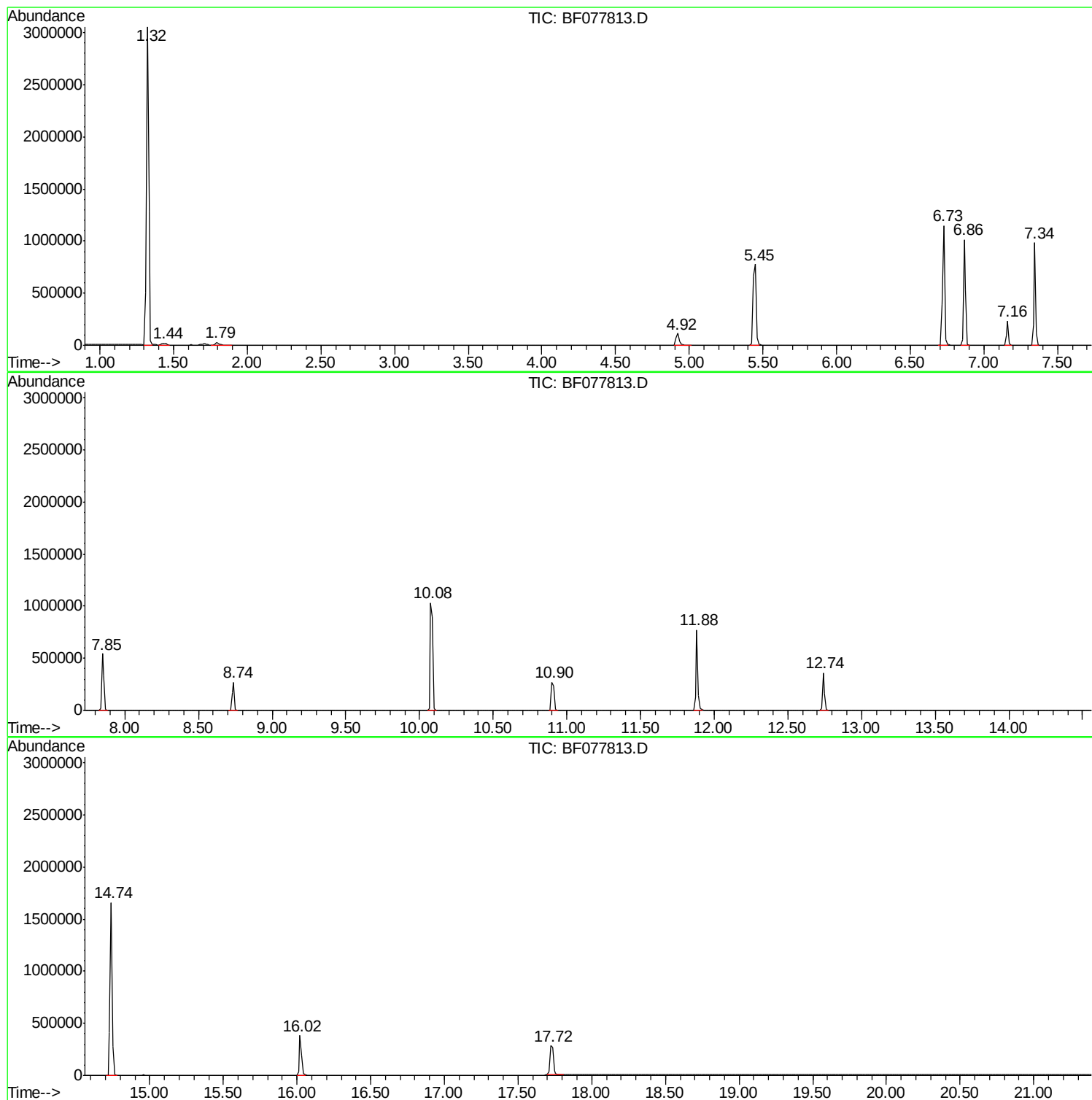
Sum of corrected areas: 14219567

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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF031115.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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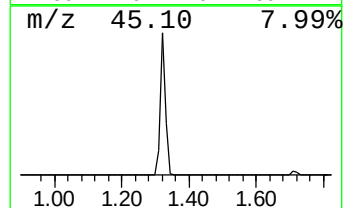
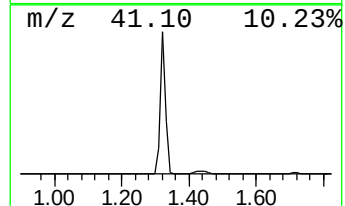
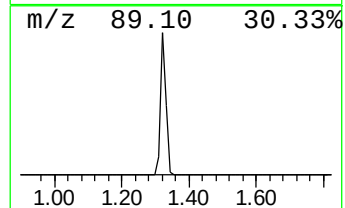
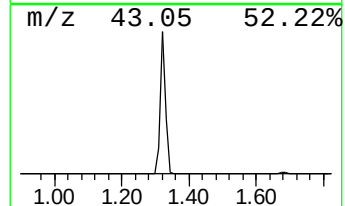
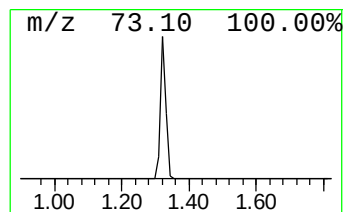
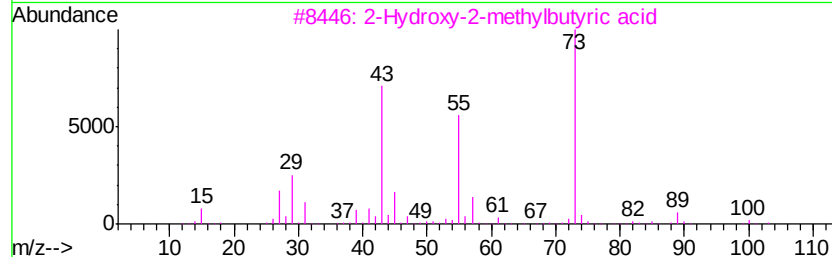
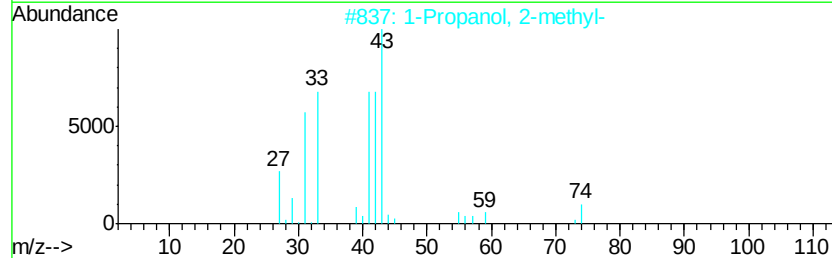
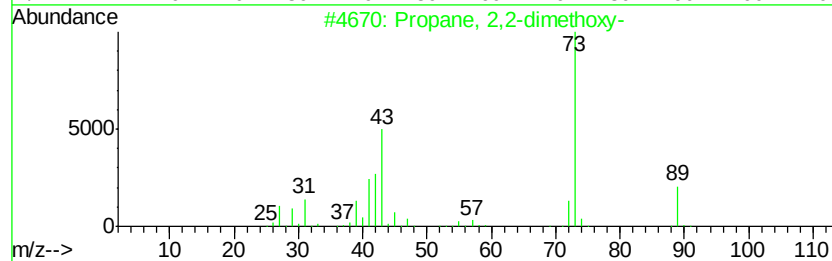
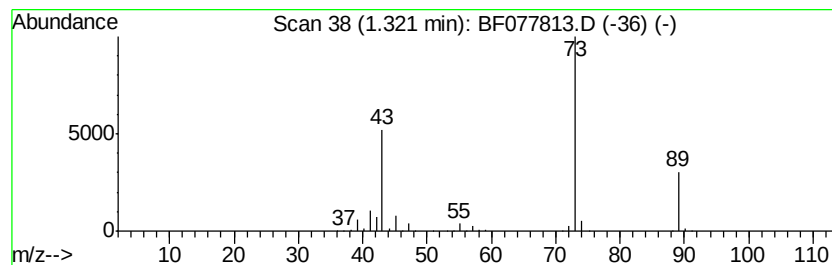
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown1.32 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 1.32 | 281.03 ng | 3347540 | 1,4-Dichlorobenzene-d4 | 7.16 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-        | 104 | C5H12O2 | 000077-76-9 | 38   |
| 2    |    | 1-Propanol, 2-methyl-          | 74  | C4H10O  | 000078-83-1 | 9    |
| 3    |    | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9    |
| 4    |    | Propane, 2-methoxy-2-methyl-   | 88  | C5H12O  | 001634-04-4 | 9    |
| 5    |    | Pentane, 3-methoxy-            | 102 | C6H14O  | 036839-67-5 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF031115.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

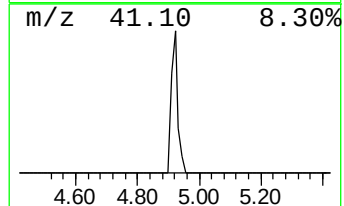
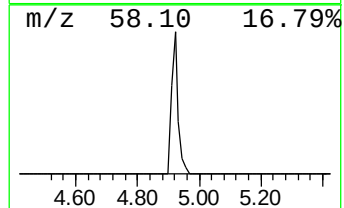
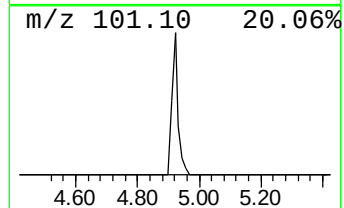
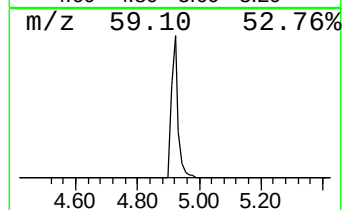
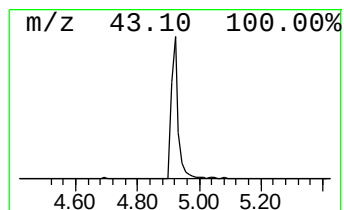
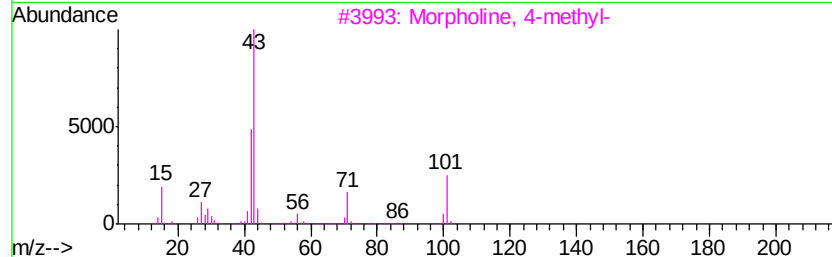
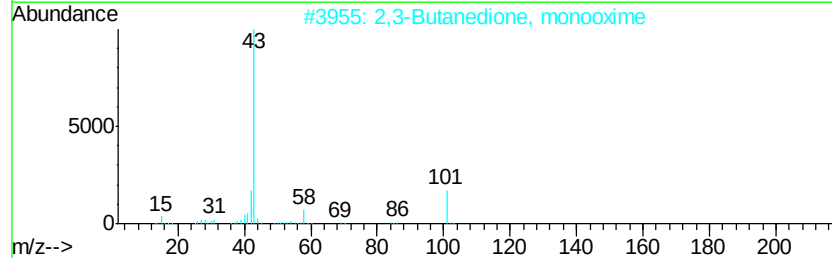
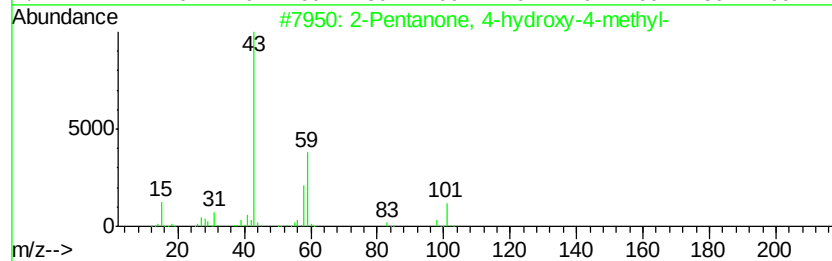
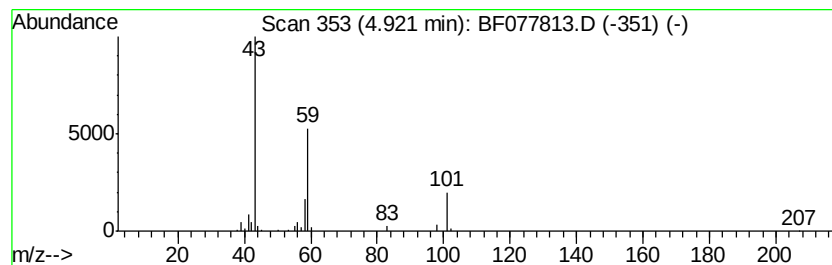
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Peak Number 4 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.92 | 13.96 ng | 166312 | 1,4-Dichlorobenzene-d4 | 7.16 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 53   |
| 2    |    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 25   |
| 3    |    | Morpholine, 4-methyl-            | 101 | C5H11NO | 000109-02-4 | 9    |
| 4    |    | 5-Hexen-2-one                    | 98  | C6H10O  | 000109-49-9 | 9    |
| 5    |    | 3-Hexanol, 4-methyl-             | 116 | C7H16O  | 000615-29-2 | 9    |



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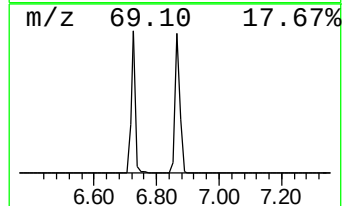
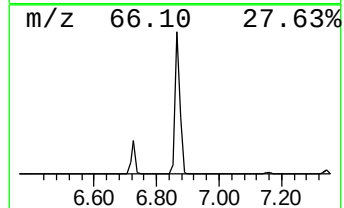
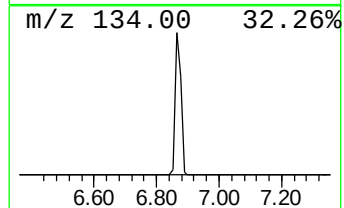
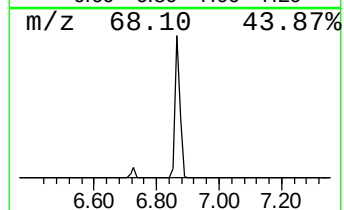
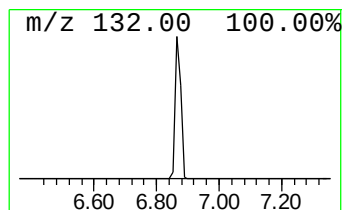
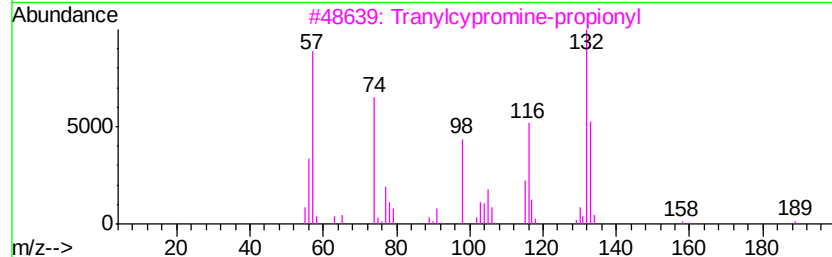
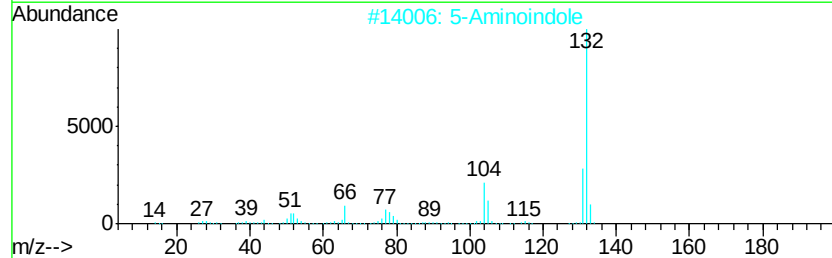
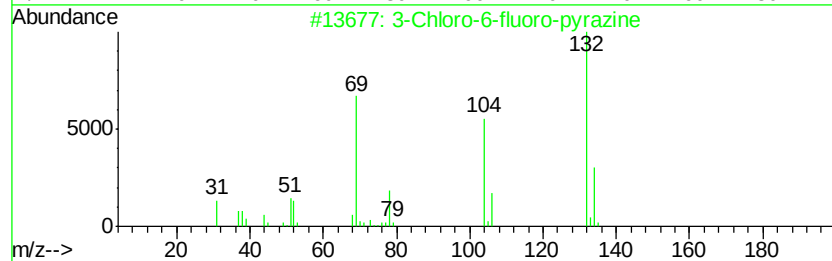
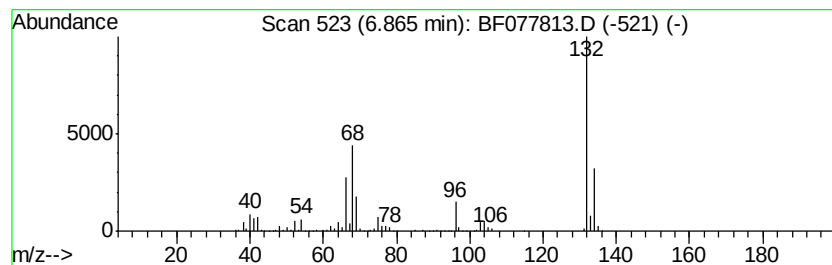
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF031115.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown6.86 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.86 | 92.96 ng | 1107330 | 1,4-Dichlorobenzene-d4 | 7.16 |

| Hit# | of                                  | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-----------|--------------|------|------|
| 1    | 3-Chloro-6-fluoro-pyrazine          | 132          | C4H2ClFN2 | 1000146-10-7 | 35   |      |
| 2    | 5-Aminoindole                       | 132          | C8H8N2    | 005192-03-0  | 12   |      |
| 3    | Tranvlcyproline-propionyl           | 189          | C12H15NO  | 1000123-86-3 | 10   |      |
| 4    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132          | C10H12    | 028749-81-7  | 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 |
| unknown1.32          | 1.32 | 281.0   | ng    | 3347540  | 1                     | 7.16 | 238233 | 20.0 |
| 2-Pentanone, 4-hy... | 4.92 | 14.0    | ng    | 166312   | 1                     | 7.16 | 238233 | 20.0 |
| unknown6.86          | 6.86 | 93.0    | ng    | 1107330  | 1                     | 7.16 | 238233 | 20.0 |