

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081916\  
 Data File : BF089817.D  
 Acq On : 20 Aug 2016 00:52  
 Operator : UM/SJ  
 Sample : H4518-14  
 Misc :  
 ALS Vial : 33 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 B-2(0-5)

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:\HPCHEM1\BNA\_F\METHODS\8270-BF081916.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         | 1.667       | 5             | 7           | 15           | rVV      | 938300         | 2217824       | 8.03%           | 1.537%        |
| 2         | 1.781       | 15            | 17          | 66           | rVB      | 10397343       | 27628996      | 100.00%         | 19.152%       |
| 3         | 4.261       | 232           | 234         | 237          | rVB      | 193429         | 280951        | 1.02%           | 0.195%        |
| 4         | 4.821       | 280           | 283         | 286          | rBV      | 2401464        | 3313046       | 11.99%          | 2.297%        |
| 5         | 5.267       | 319           | 322         | 324          | rBV      | 9563025        | 9960427       | 36.05%          | 6.904%        |
| 6         | 6.319       | 411           | 414         | 417          | rBV      | 7643060        | 8843333       | 32.01%          | 6.130%        |
| 7         | 6.444       | 423           | 425         | 428          | rBV      | 8374100        | 9822602       | 35.55%          | 6.809%        |
| 8         | 6.685       | 444           | 446         | 448          | rBV      | 4116456        | 3319624       | 12.02%          | 2.301%        |
| 9         | 6.845       | 457           | 460         | 462          | rBV      | 8164451        | 8814085       | 31.90%          | 6.110%        |
| 10        | 7.245       | 493           | 495         | 498          | rBV      | 4876758        | 5977975       | 21.64%          | 4.144%        |
| 11        | 7.965       | 556           | 558         | 561          | rBV      | 3975025        | 4013768       | 14.53%          | 2.782%        |
| 12        | 9.050       | 650           | 653         | 655          | rBV      | 12674988       | 11626670      | 42.08%          | 8.059%        |
| 13        | 9.439       | 685           | 687         | 690          | rBV      | 1955419        | 2012050       | 7.28%           | 1.395%        |
| 14        | 9.713       | 709           | 711         | 713          | rBV      | 4436823        | 4108112       | 14.87%          | 2.848%        |
| 15        | 9.748       | 713           | 714         | 716          | rVB      | 460933         | 331625        | 1.20%           | 0.230%        |
| 16        | 10.502      | 777           | 780         | 782          | rVV      | 4566717        | 5241796       | 18.97%          | 3.633%        |
| 17        | 10.639      | 790           | 792         | 796          | rVB      | 353744         | 429880        | 1.56%           | 0.298%        |
| 18        | 11.188      | 838           | 840         | 844          | rBV2     | 3564192        | 5616694       | 20.33%          | 3.893%        |
| 19        | 11.268      | 844           | 847         | 848          | rVB      | 458625         | 544887        | 1.97%           | 0.378%        |
| 20        | 11.714      | 885           | 886         | 887          | rVV      | 261688         | 304432        | 1.10%           | 0.211%        |
| 21        | 11.748      | 887           | 889         | 892          | rVV2     | 225949         | 517481        | 1.87%           | 0.359%        |
| 22        | 11.805      | 892           | 894         | 898          | rVB2     | 351565         | 608959        | 2.20%           | 0.422%        |
| 23        | 11.988      | 908           | 910         | 914          | rVB2     | 204856         | 293273        | 1.06%           | 0.203%        |
| 24        | 12.399      | 943           | 946         | 948          | rVV      | 2360909        | 2500658       | 9.05%           | 1.733%        |
| 25        | 12.525      | 955           | 957         | 962          | rBV4     | 237489         | 436822        | 1.58%           | 0.303%        |
| 26        | 12.617      | 962           | 965         | 967          | rVV2     | 2100706        | 2645358       | 9.57%           | 1.834%        |
| 27        | 12.777      | 977           | 979         | 982          | rVB      | 6087370        | 7105253       | 25.72%          | 4.925%        |
| 28        | 12.959      | 991           | 995         | 996          | rVB3     | 187047         | 405156        | 1.47%           | 0.281%        |
| 29        | 13.748      | 1062          | 1064        | 1069         | rBV5     | 210762         | 435942        | 1.58%           | 0.302%        |
| 30        | 13.851      | 1070          | 1073        | 1077         | rVV2     | 3004975        | 5263869       | 19.05%          | 3.649%        |
| 31        | 14.960      | 1167          | 1170        | 1175         | rBV      | 1129309        | 2216930       | 8.02%           | 1.537%        |
| 32        | 15.234      | 1192          | 1194        | 1197         | rVB      | 701975         | 811991        | 2.94%           | 0.563%        |
| 33        | 15.291      | 1197          | 1199        | 1201         | rVV      | 1069239        | 1155486       | 4.18%           | 0.801%        |
| 34        | 15.348      | 1201          | 1204        | 1211         | rVB      | 2844511        | 3583142       | 12.97%          | 2.484%        |

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BNA\_F  
ClientSampleId :  
B-2(0-5)

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-BF081916.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |       |        |
|----|--------|------|------|------|------|--------|--------|-------|--------|
| 35 | 16.628 | 1314 | 1316 | 1321 | rVB2 | 399752 | 783134 | 2.83% | 0.543% |
| 36 | 17.017 | 1347 | 1350 | 1358 | rVB  | 377301 | 799960 | 2.90% | 0.555% |
| 37 | 17.223 | 1365 | 1368 | 1376 | rVB2 | 113430 | 291755 | 1.06% | 0.202% |

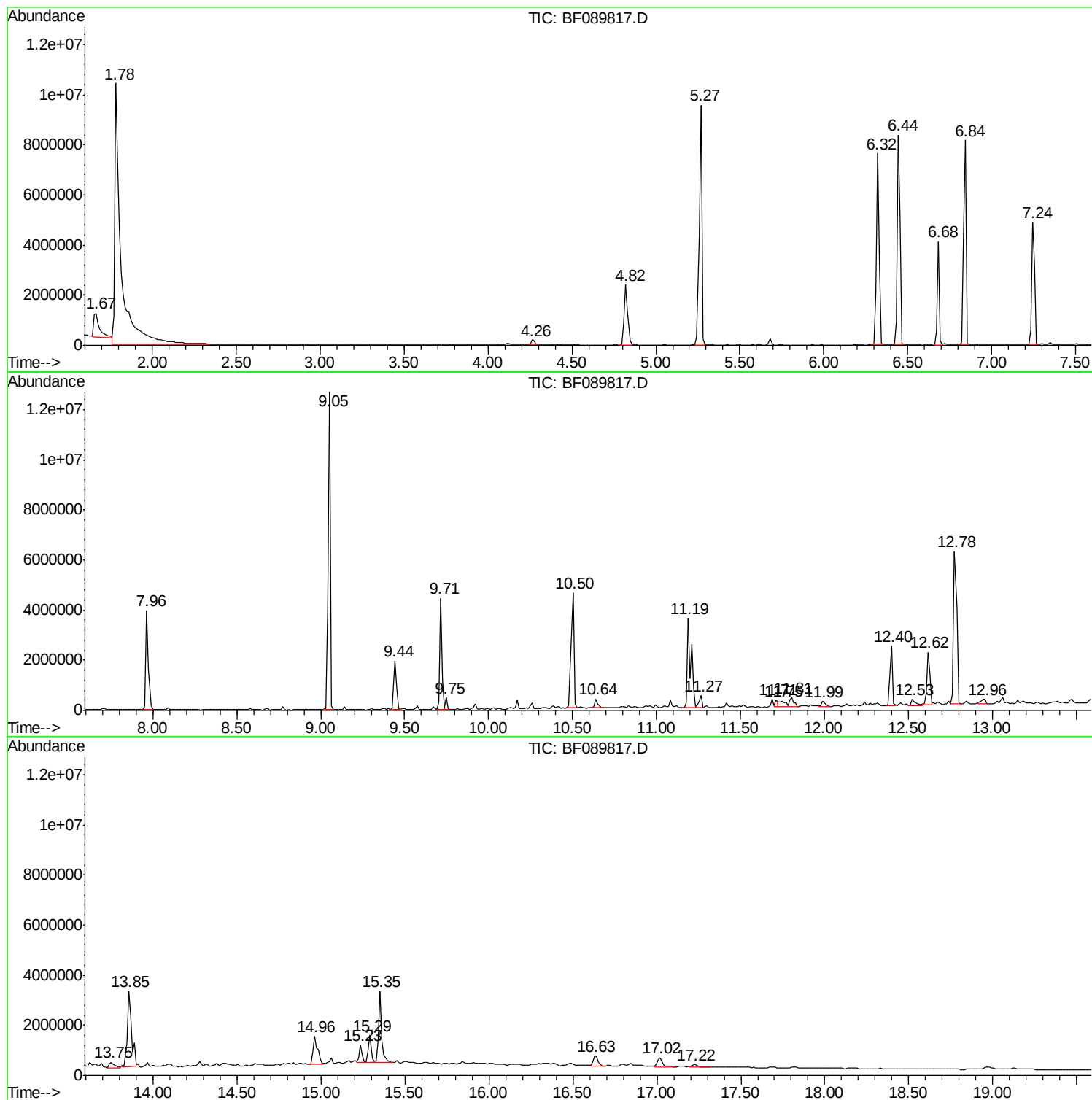
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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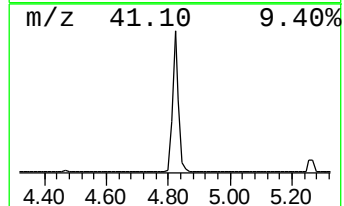
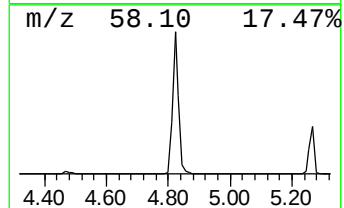
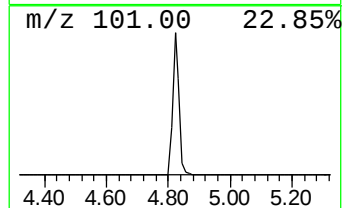
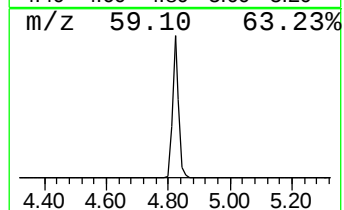
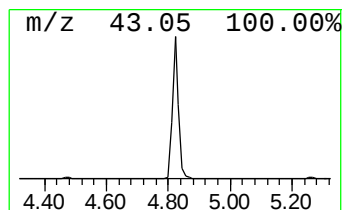
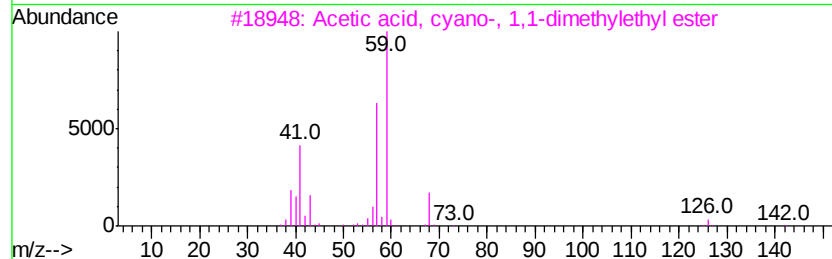
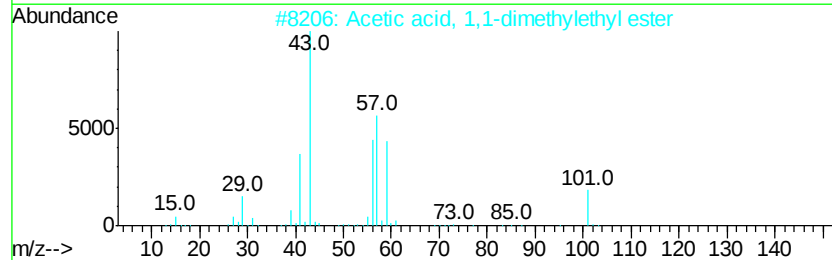
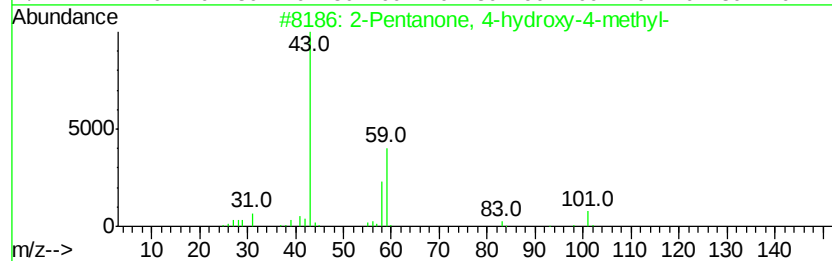
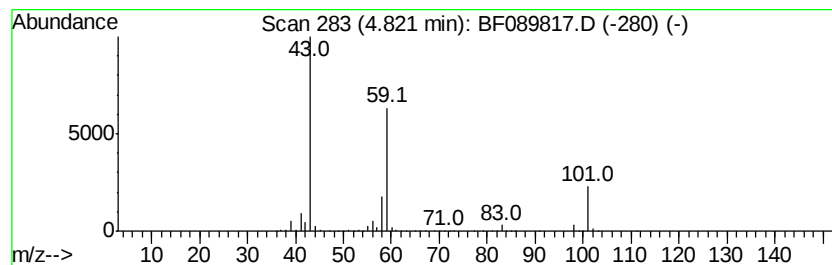
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.82 | 19.96 ng | 3313050 | 1,4-Dichlorobenzene-d4 | 6.68 |

| 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, 1,1-dimethylethyl e...  | 116 | C6H12O2  | 000540-88-5 | 39   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 4    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f...   | 101 | C4H7NO2  | 016504-58-8 | 9    |
| 5    |    | Acetone                              | 58  | C3H6O    | 000067-64-1 | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081916.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

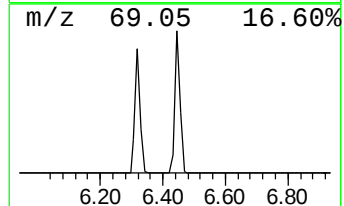
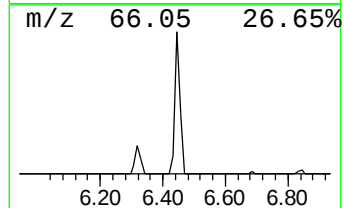
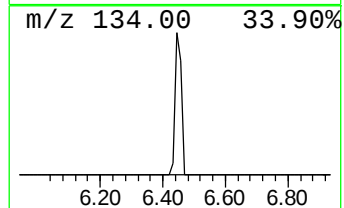
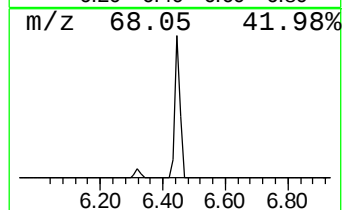
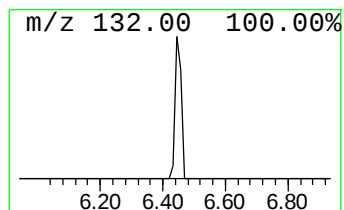
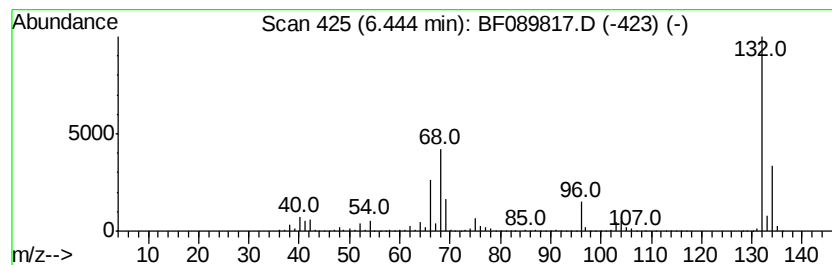
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown6.44 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.44 | 59.18 ng | 9822600 | 1,4-Dichlorobenzene-d4 | 6.68 |

| Hit# | of    | Tentative ID               | MW  | MolForm   | CAS#         | Qual |
|------|-------|----------------------------|-----|-----------|--------------|------|
| 1    | 3     | Chloro-6-fluoro-pyrazine   | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    | (E)-3 | Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 27   |
| 3    | 5     | Aminoindole                | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    | 4     | Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6  | 9    |
| 5    | 5     | Fluoro-2-chloropyrimidine  | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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Instrument :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081916.M  
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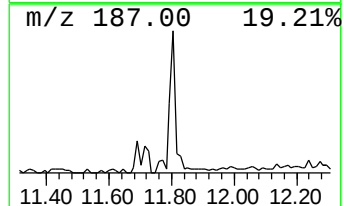
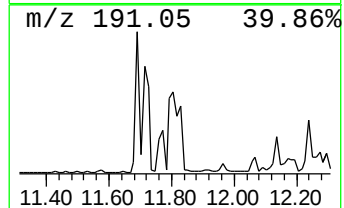
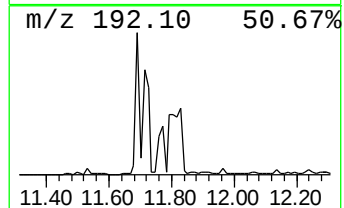
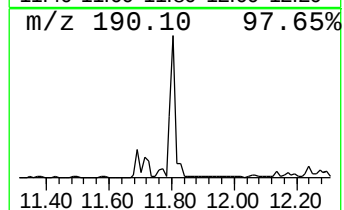
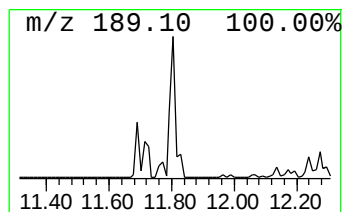
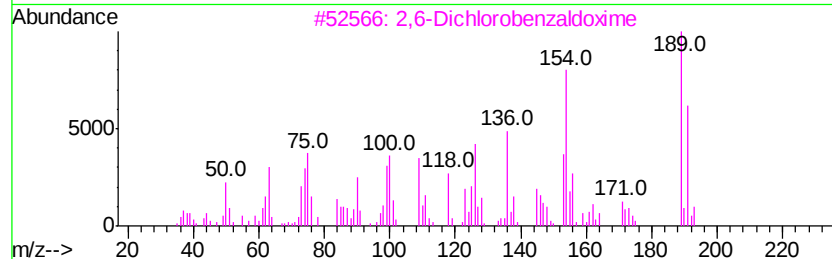
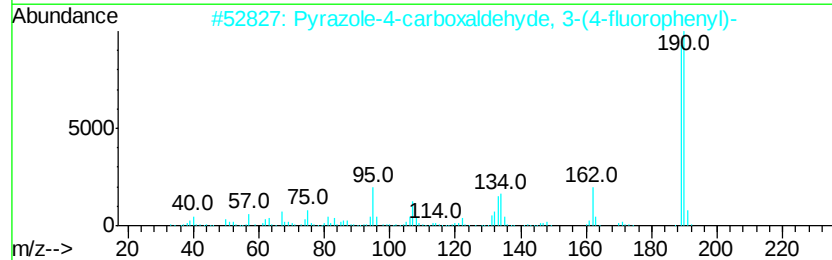
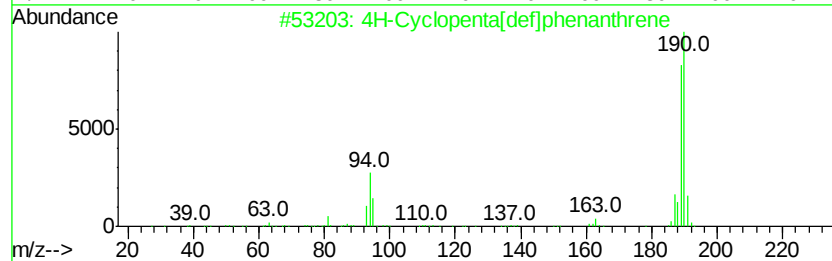
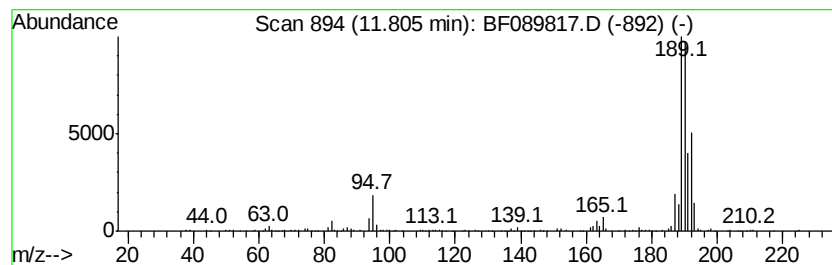
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.81 | 2.17 ng | 608959 | Phenanthrene-d10 | 11.19 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 4H-Cyclopenta[def]phenanthrene      | 190 | C15H10    | 000203-64-5 | 92   |
| 2    |    |   | Pyrazole-4-carboxaldehyde, 3-(4-... | 190 | C10H7FN2O | 306936-57-2 | 49   |
| 3    |    |   | 2,6-Dichlorobenzaloxime             | 189 | C7H5Cl2NO | 025185-95-9 | 38   |
| 4    |    |   | 1H-Indene, 2-phenyl-                | 192 | C15H12    | 004505-48-0 | 22   |
| 5    |    |   | Anthracene, 9-methyl-               | 192 | C15H12    | 000779-02-2 | 22   |



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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... | 4.82  | 20.0    | ng    | 3313050  | 1                     | 6.68  | 3319620 | 20.0 |
| unknown6.44          | 6.44  | 59.2    | ng    | 9822600  | 1                     | 6.68  | 3319620 | 20.0 |
| 4H-Cyclopenta[def... | 11.81 | 2.2     | ng    | 608959   | 4                     | 11.19 | 5616690 | 20.0 |