

Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG092316\  
 Data File : BG024091.D  
 Acq On : 23 Sep 2016 17:30  
 Operator : UM/SJ  
 Sample : H4803-03  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PT-BN-WP

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\_G\METHODS\8270-BG092316.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         | 2.902       | 7             | 11          | 27           | rVB      | 5041231        | 7667323       | 66.65%          | 5.944%        |
| 2         | 5.105       | 381           | 386         | 394          | rBV      | 172998         | 255610        | 2.22%           | 0.198%        |
| 3         | 5.586       | 463           | 468         | 480          | rBV      | 857982         | 1464480       | 12.73%          | 1.135%        |
| 4         | 7.213       | 738           | 745         | 757          | rBV      | 986808         | 1766217       | 15.35%          | 1.369%        |
| 5         | 7.454       | 780           | 786         | 793          | rVB      | 916113         | 1447432       | 12.58%          | 1.122%        |
| 6         | 7.572       | 800           | 806         | 815          | rBV      | 897850         | 1596445       | 13.88%          | 1.238%        |
| 7         | 7.924       | 859           | 866         | 878          | rVV      | 1318658        | 2274623       | 19.77%          | 1.763%        |
| 8         | 8.042       | 880           | 886         | 887          | rVV      | 188383         | 258252        | 2.24%           | 0.200%        |
| 9         | 8.077       | 887           | 892         | 899          | rVB      | 612517         | 1079325       | 9.38%           | 0.837%        |
| 10        | 8.365       | 934           | 941         | 943          | rBV      | 691760         | 1102899       | 9.59%           | 0.855%        |
| 11        | 8.394       | 943           | 946         | 955          | rVB      | 911867         | 1583277       | 13.76%          | 1.227%        |
| 12        | 9.223       | 1080          | 1087        | 1091         | rBV      | 638629         | 1196278       | 10.40%          | 0.927%        |
| 13        | 9.264       | 1091          | 1094        | 1108         | rVB      | 360030         | 652886        | 5.68%           | 0.506%        |
| 14        | 9.781       | 1174          | 1182        | 1190         | rBV      | 276088         | 493665        | 4.29%           | 0.383%        |
| 15        | 10.873      | 1362          | 1368        | 1372         | rBV      | 256140         | 449488        | 3.91%           | 0.348%        |
| 16        | 10.926      | 1372          | 1377        | 1387         | rVB      | 255348         | 479792        | 4.17%           | 0.372%        |
| 17        | 11.196      | 1415          | 1423        | 1432         | rVB      | 1011175        | 1733351       | 15.07%          | 1.344%        |
| 18        | 12.536      | 1643          | 1651        | 1663         | rBV      | 1240154        | 2120915       | 18.44%          | 1.644%        |
| 19        | 13.329      | 1779          | 1786        | 1796         | rBV      | 1891286        | 2874302       | 24.98%          | 2.228%        |
| 20        | 14.163      | 1921          | 1928        | 1940         | rBV      | 1937985        | 2933765       | 25.50%          | 2.274%        |
| 21        | 14.445      | 1967          | 1976        | 1985         | rBV      | 3039600        | 4994793       | 43.42%          | 3.872%        |
| 22        | 14.715      | 2015          | 2022        | 2027         | rBV      | 492312         | 769223        | 6.69%           | 0.596%        |
| 23        | 14.780      | 2027          | 2033        | 2043         | rVB      | 1610954        | 2611071       | 22.70%          | 2.024%        |
| 24        | 15.532      | 2154          | 2161        | 2170         | rBV      | 2299904        | 3185816       | 27.69%          | 2.470%        |
| 25        | 15.767      | 2193          | 2201        | 2210         | rBV2     | 5190192        | 11504415      | 100.00%         | 8.919%        |
| 26        | 16.219      | 2272          | 2278        | 2289         | rBV      | 1696590        | 2666747       | 23.18%          | 2.067%        |
| 27        | 16.660      | 2346          | 2353        | 2364         | rBV      | 3977470        | 5724653       | 49.76%          | 4.438%        |
| 28        | 16.789      | 2368          | 2375        | 2384         | rVV      | 2342428        | 3379028       | 29.37%          | 2.620%        |
| 29        | 17.482      | 2486          | 2493        | 2503         | rBV2     | 666992         | 1024568       | 8.91%           | 0.794%        |
| 30        | 17.623      | 2507          | 2517        | 2528         | rBV      | 1893097        | 2985592       | 25.95%          | 2.315%        |
| 31        | 18.434      | 2648          | 2655        | 2662         | rBV      | 2132092        | 2737413       | 23.79%          | 2.122%        |
| 32        | 18.921      | 2733          | 2738        | 2750         | rVB      | 250446         | 420962        | 3.66%           | 0.326%        |
| 33        | 19.550      | 2837          | 2845        | 2854         | rBV      | 5719176        | 8698756       | 75.61%          | 6.744%        |
| 34        | 19.879      | 2895          | 2901        | 2910         | rBV      | 118536         | 189941        | 1.65%           | 0.147%        |

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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

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\_G\METHODS\8270-BG092316.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 35 | 20.096 | 2932 | 2938 | 2945 | rBV  | 3695320 | 4855675 | 42.21% | 3.765% |
| 36 | 20.783 | 3048 | 3055 | 3063 | rBV  | 4709024 | 6033714 | 52.45% | 4.678% |
| 37 | 21.641 | 3195 | 3201 | 3207 | rBV  | 1843027 | 2606694 | 22.66% | 2.021% |
| 38 | 21.776 | 3216 | 3224 | 3230 | rBV2 | 1645585 | 3680418 | 31.99% | 2.853% |
| 39 | 21.847 | 3230 | 3236 | 3248 | rVB  | 3102975 | 5165080 | 44.90% | 4.004% |
| 40 | 24.073 | 3604 | 3615 | 3626 | rBV  | 1669499 | 4114656 | 35.77% | 3.190% |
| 41 | 24.995 | 3757 | 3772 | 3781 | rBV  | 2409454 | 7254556 | 63.06% | 5.624% |
| 42 | 25.130 | 3786 | 3795 | 3807 | rVB3 | 323268  | 1055519 | 9.17%  | 0.818% |
| 43 | 28.966 | 4431 | 4448 | 4463 | rVB2 | 864602  | 3707001 | 32.22% | 2.874% |
| 44 | 30.200 | 4631 | 4658 | 4674 | rBV  | 1134457 | 6188940 | 53.80% | 4.798% |

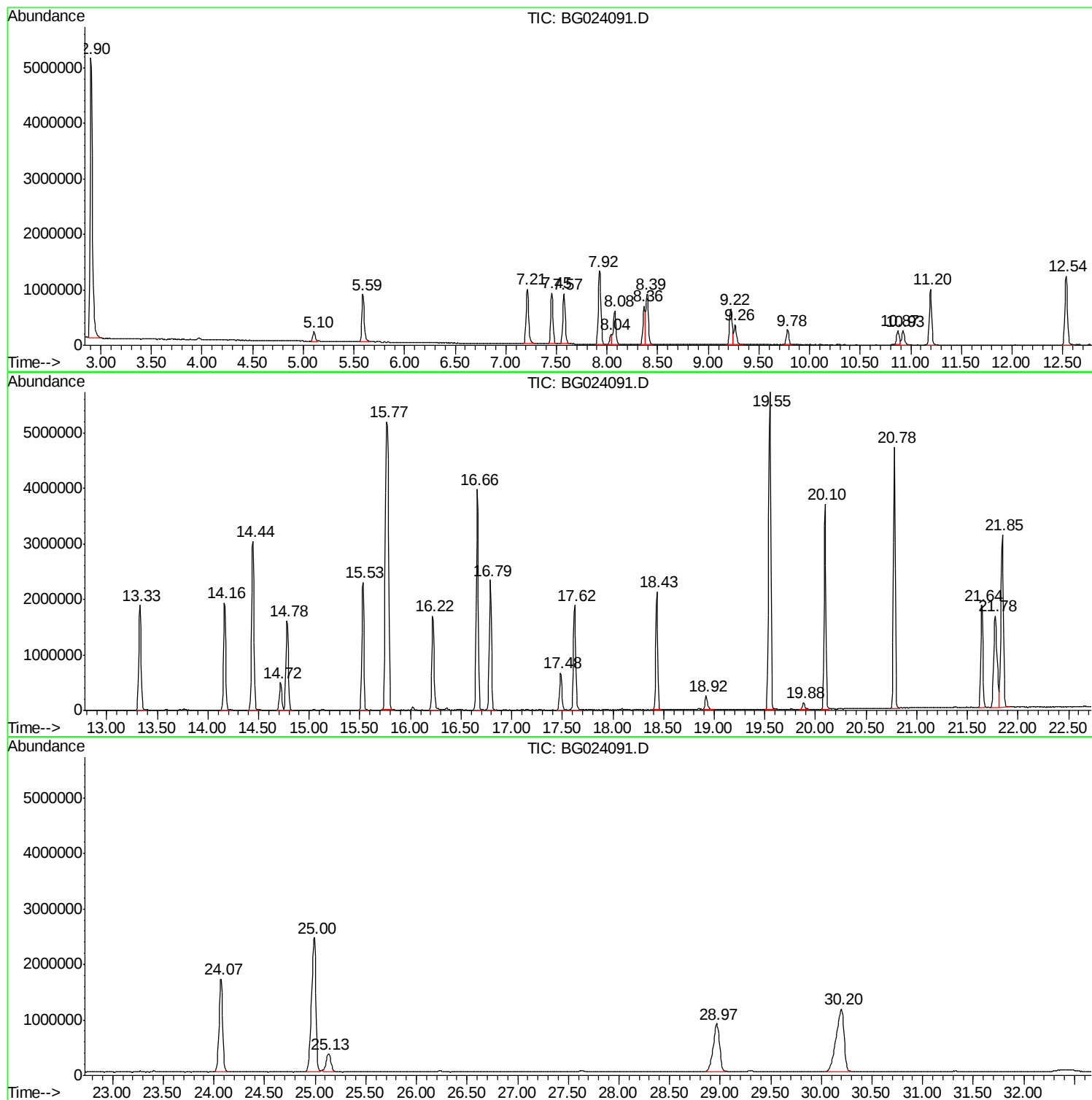
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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG092316\  
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Acq On : 23 Sep 2016 17:30  
Operator : UM/SJ  
Sample : H4803-03  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

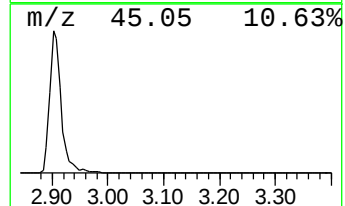
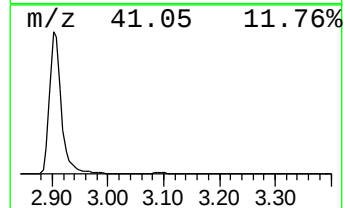
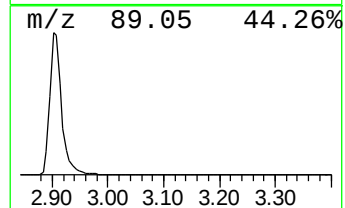
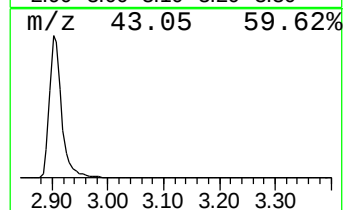
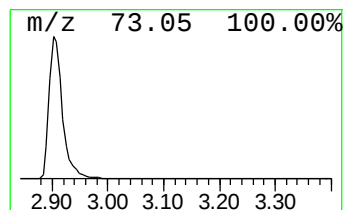
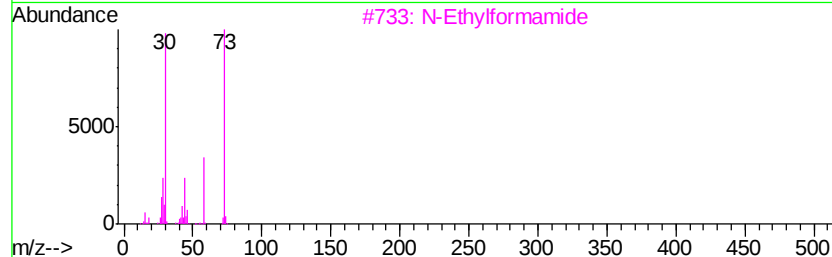
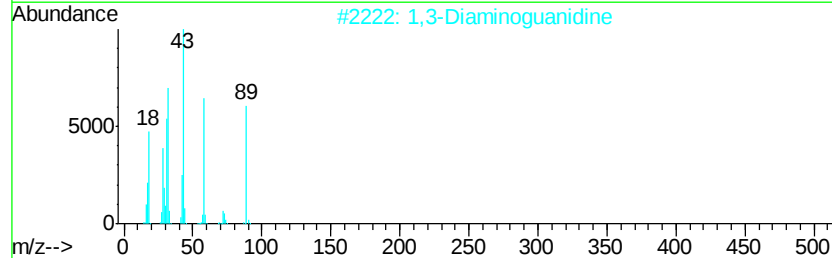
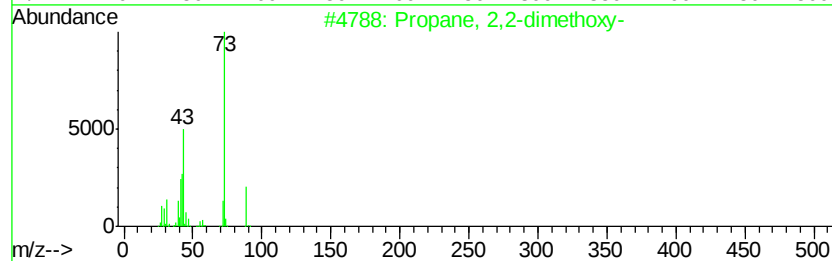
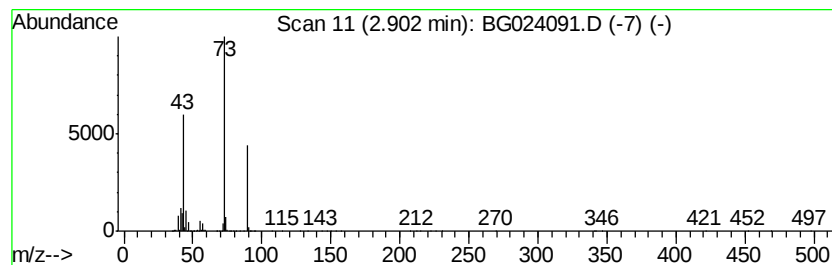
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.90 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 2.90 | 593.79 ng | 7667320 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | Propane, 2,2-dimethoxy-        | 104 | C5H12O2 | 000077-76-9 | 40   |
| 2    |    | 1,3-Diaminoguanidine           | 89  | CH7N5   | 004364-78-7 | 23   |
| 3    |    | N-Ethylformamide               | 73  | C3H7NO  | 000627-45-2 | 9    |
| 4    |    | 1-Propanol, 2-methyl-2-nitro-  | 119 | C4H9NO3 | 000076-39-1 | 9    |
| 5    |    | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

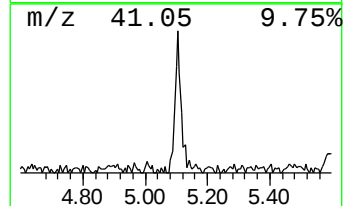
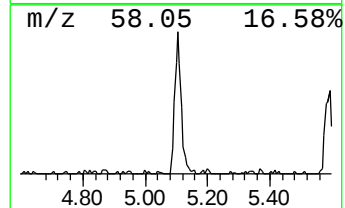
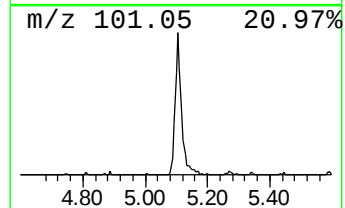
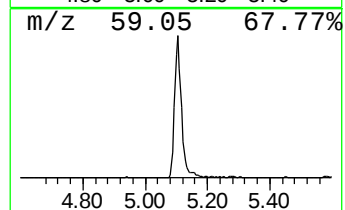
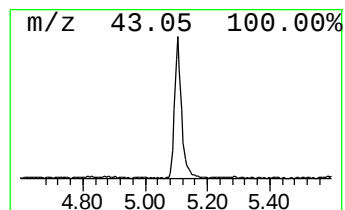
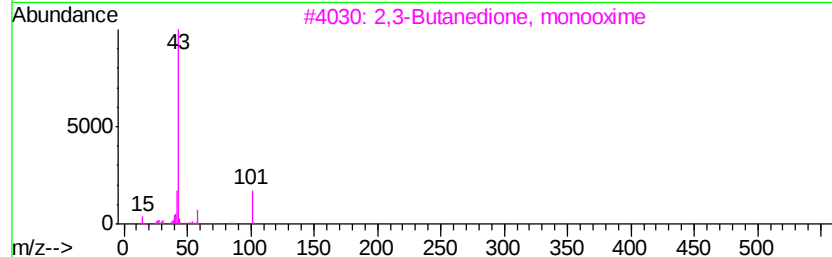
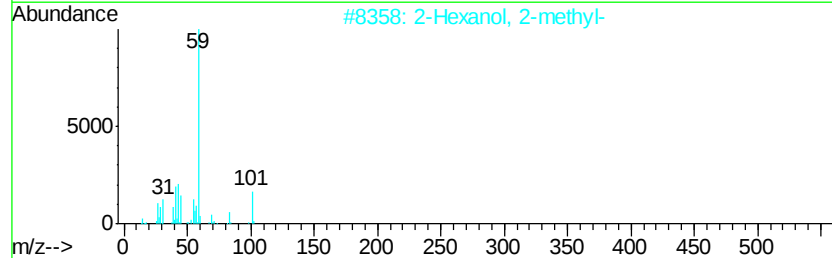
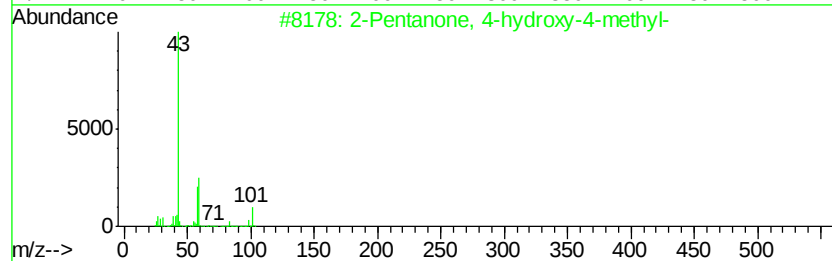
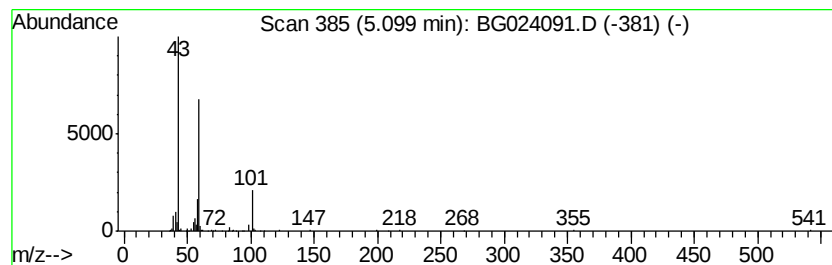
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.10 | 19.80 ng | 255610 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 45   |
| 2    |    | 2-Hexanol, 2-methyl-             | 116 | C7H16O  | 000625-23-0 | 37   |
| 3    |    | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6 | 25   |
| 4    |    | 3-Hexanol, 4-methyl-             | 116 | C7H16O  | 000615-29-2 | 23   |
| 5    |    | 3-Hydroxy-3-methyl-2-butanone    | 102 | C5H10O2 | 000115-22-0 | 12   |



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Misc :  
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Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

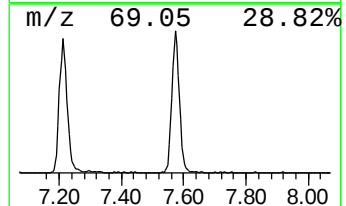
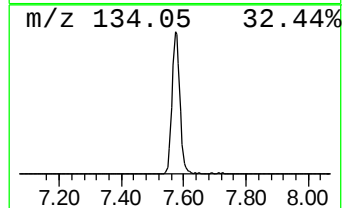
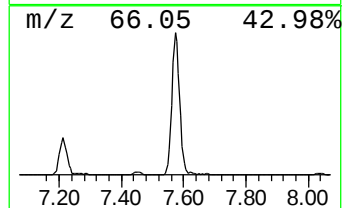
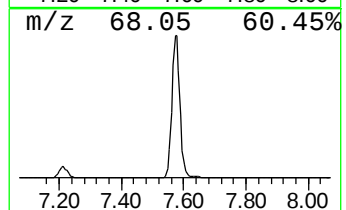
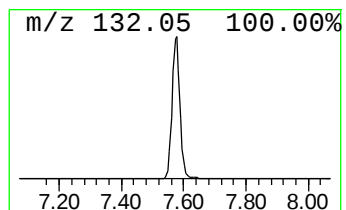
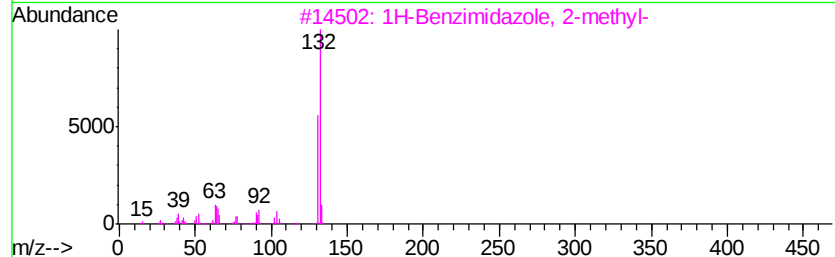
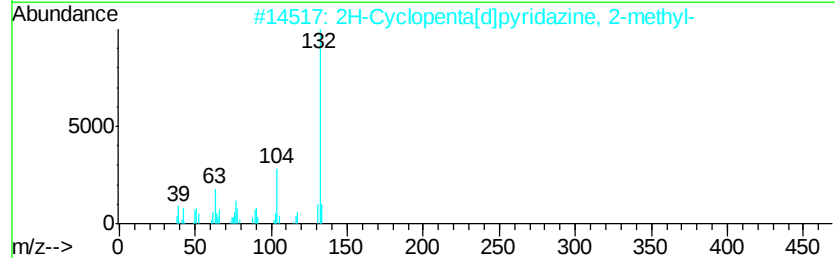
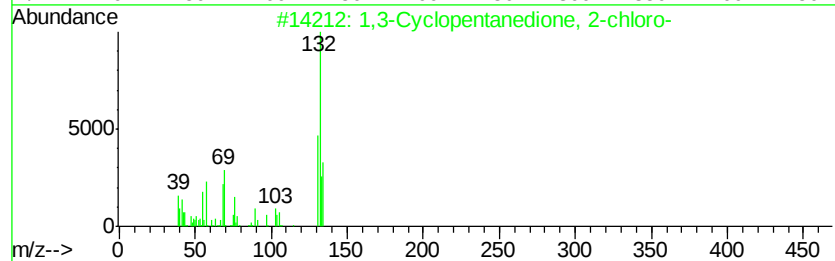
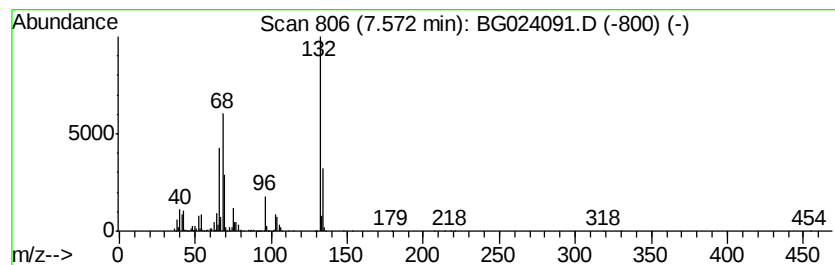
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown7.57 Concentration Rank 2

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.57 | 123.64 ng | 1596450 | 1,4-Dichlorobenzene-d4 | 8.04 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 1,3-Cyclopentanedione, 2-chloro-    | 132 | C5H5ClO2  | 014203-19-1  | 27   |
| 2    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 18   |
| 3    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6  | 14   |
| 4    |    | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 14   |



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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

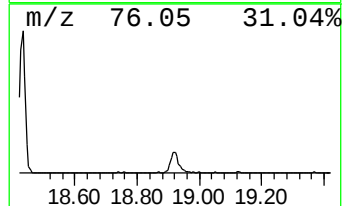
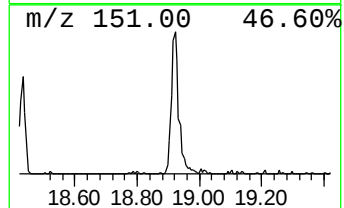
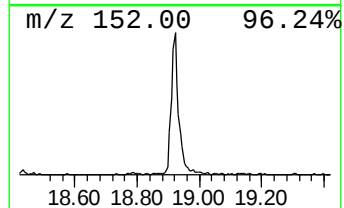
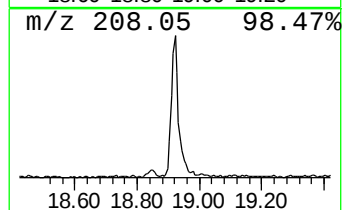
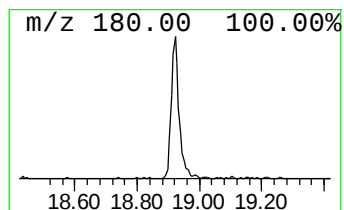
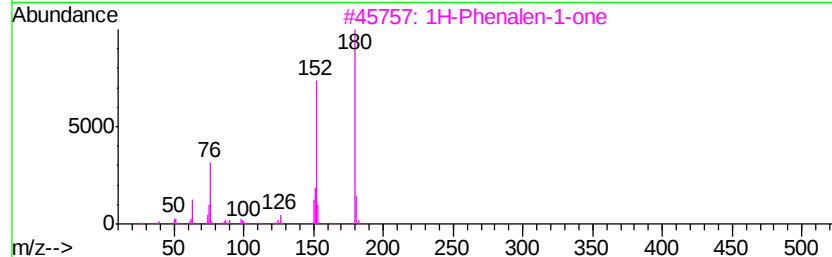
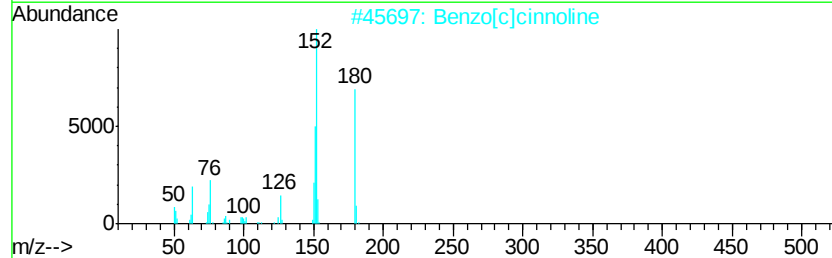
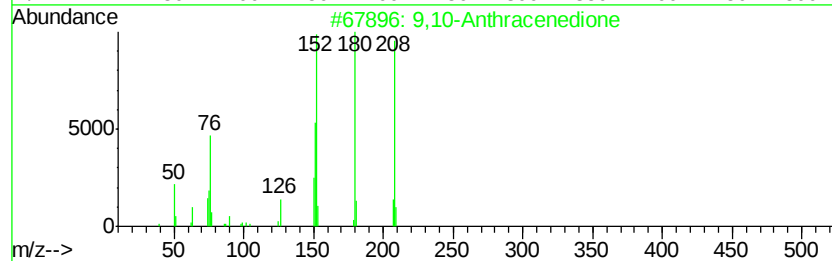
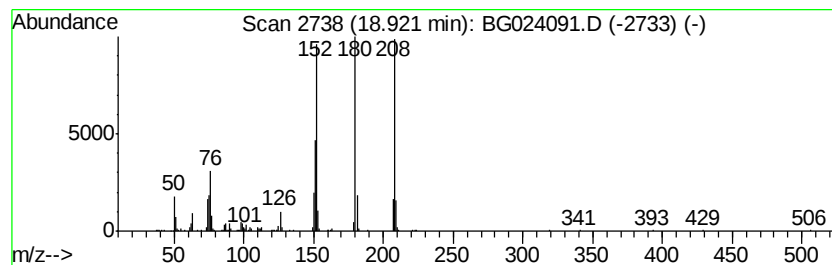
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 9,10-Anthracenedione Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.92 | 8.22 ng | 420962 | Phenanthrene-d10 | 17.48 |

| Hit# | of | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------|-----|---------|-------------|------|
| 1    | 5  | 9,10-Anthracenedione | 208 | C14H8O2 | 000084-65-1 | 97   |
| 2    |    | Benzo[c]cinnoline    | 180 | C12H8N2 | 000230-17-1 | 64   |
| 3    |    | 1H-Phenalen-1-one    | 180 | C13H8O  | 000548-39-0 | 60   |
| 4    |    | 1,4-Anthracenedione  | 208 | C14H8O2 | 000635-12-1 | 58   |
| 5    |    | 9H-Fluoren-9-one     | 180 | C13H8O  | 000486-25-9 | 58   |



Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG092316\  
Data File : BG024091.D  
Acq On : 23 Sep 2016 17:30  
Operator : UM/SJ  
Sample : H4803-03  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PT-BN-WP

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG092316.M  
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 |
| unknown2.90          | 2.90  | 593.8   | ng    | 7667320  | 1                     | 8.04  | 258252  | 20.0 |
| 2-Pentanone, 4-hy... | 5.10  | 19.8    | ng    | 255610   | 1                     | 8.04  | 258252  | 20.0 |
| unknown7.57          | 7.57  | 123.6   | ng    | 1596450  | 1                     | 8.04  | 258252  | 20.0 |
| 9,10-Anthracenedione | 18.92 | 8.2     | ng    | 420962   | 4                     | 17.48 | 1024570 | 20.0 |