

Data Path : S:\HPCHEM1\BNA\_G\DATA\BG120817\  
 Data File : BG031421.D  
 Acq On : 8 Dec 2017 13:34  
 Operator : SJ/JU  
 Sample : I6717-04  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 PB-3(10-20)

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-BG111017.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         | 5.199       | 321           | 325         | 335          | rVB      | 54504          | 89747         | 1.62%           | 0.357%        |
| 2         | 5.681       | 400           | 407         | 425          | rBV      | 805908         | 1437954       | 25.93%          | 5.718%        |
| 3         | 7.291       | 674           | 681         | 699          | rBV      | 904437         | 1700644       | 30.67%          | 6.763%        |
| 4         | 7.661       | 736           | 744         | 754          | rBV      | 879310         | 1610616       | 29.05%          | 6.405%        |
| 5         | 8.125       | 815           | 823         | 832          | rBV      | 151821         | 259762        | 4.68%           | 1.033%        |
| 6         | 8.449       | 870           | 878         | 889          | rBV      | 676395         | 1225470       | 22.10%          | 4.873%        |
| 7         | 9.295       | 1012          | 1022        | 1034         | rBV      | 510569         | 1013118       | 18.27%          | 4.029%        |
| 8         | 10.940      | 1294          | 1302        | 1320         | rBV      | 186468         | 405965        | 7.32%           | 1.614%        |
| 9         | 13.372      | 1708          | 1716        | 1738         | rBV      | 1803326        | 2946535       | 53.14%          | 11.717%       |
| 10        | 14.195      | 1849          | 1856        | 1865         | rBV      | 190843         | 345233        | 6.23%           | 1.373%        |
| 11        | 14.747      | 1944          | 1950        | 1961         | rVB2     | 427080         | 718156        | 12.95%          | 2.856%        |
| 12        | 16.234      | 2197          | 2203        | 2223         | rBV      | 1763881        | 2810743       | 50.69%          | 11.177%       |
| 13        | 16.427      | 2231          | 2236        | 2239         | rBV      | 44454          | 60400         | 1.09%           | 0.240%        |
| 14        | 17.491      | 2409          | 2417        | 2432         | rBV2     | 695363         | 1140498       | 20.57%          | 4.535%        |
| 15        | 19.753      | 2798          | 2802        | 2811         | rBV5     | 49151          | 96557         | 1.74%           | 0.384%        |
| 16        | 20.082      | 2852          | 2858        | 2865         | rVB      | 4087354        | 5544985       | 100.00%         | 22.051%       |
| 17        | 20.294      | 2891          | 2894        | 2900         | rVB      | 41763          | 63038         | 1.14%           | 0.251%        |
| 18        | 20.746      | 2966          | 2971        | 2977         | rBV      | 247614         | 427727        | 7.71%           | 1.701%        |
| 19        | 20.816      | 2977          | 2983        | 2987         | rVV2     | 175061         | 336494        | 6.07%           | 1.338%        |
| 20        | 21.762      | 3138          | 3144        | 3157         | rVB2     | 750995         | 1339206       | 24.15%          | 5.326%        |
| 21        | 23.225      | 3386          | 3393        | 3404         | rBV3     | 98986          | 241011        | 4.35%           | 0.958%        |
| 22        | 25.059      | 3692          | 3705        | 3718         | rBV2     | 420112         | 1332688       | 24.03%          | 5.300%        |

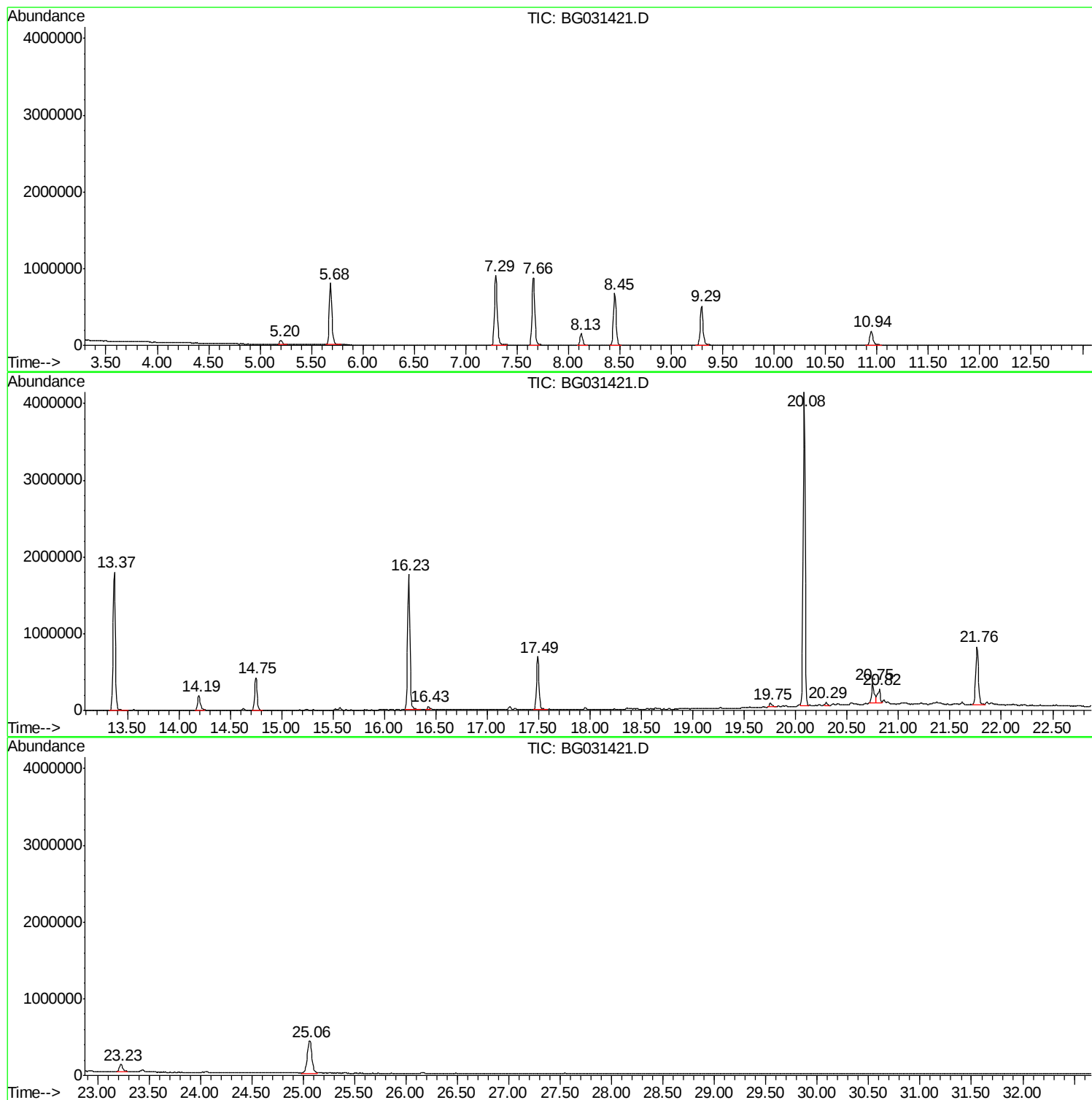
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Instrument :  
BNA\_G  
ClientSampleId :  
PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG111017.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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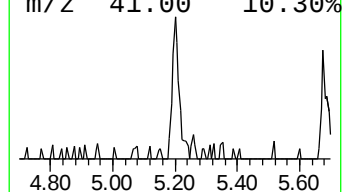
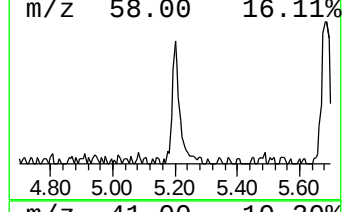
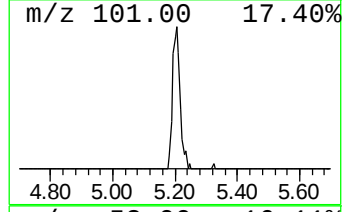
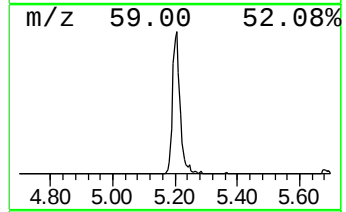
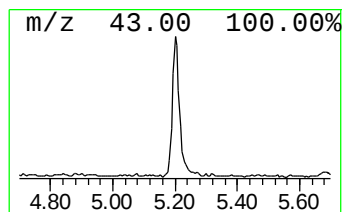
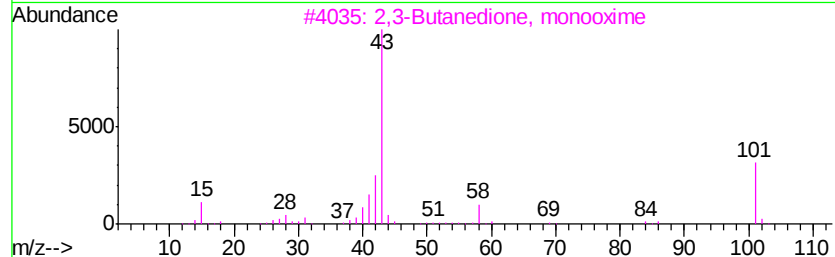
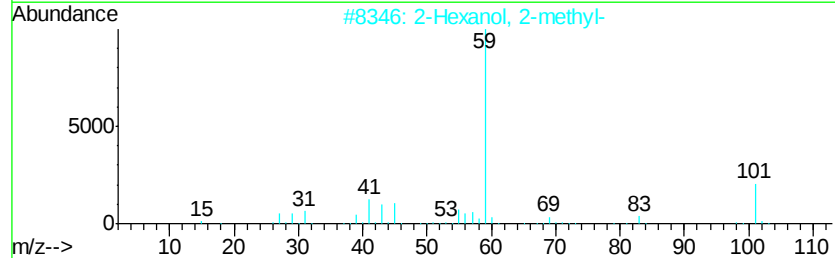
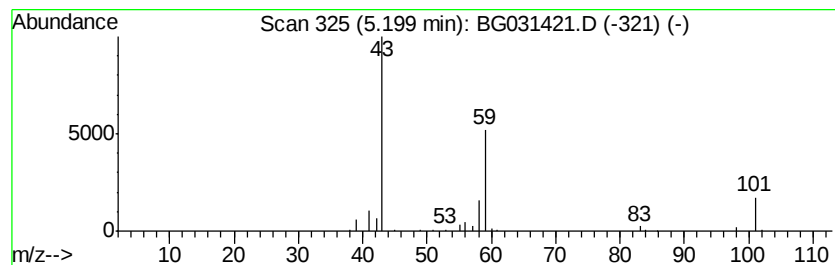
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 5.20 | 6.91 ng | 89747 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of 5 | Tentative ID                     | MW  | MolForm | CAS#         | Qual |
|------|------|----------------------------------|-----|---------|--------------|------|
| 1    |      | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2  | 50   |
| 2    |      | 2-Hexanol, 2-methyl-             | 116 | C7H16O  | 000625-23-0  | 38   |
| 3    |      | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6  | 9    |
| 4    |      | n-Propyl t-butyl ether           | 116 | C7H16O  | 1000334-81-9 | 9    |
| 5    |      | 3-Hydroxy-3-methyl-2-butanone    | 102 | C5H10O2 | 000115-22-0  | 9    |



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Instrument :  
BNA\_G  
ClientSampleId :  
PB-3(10-20)

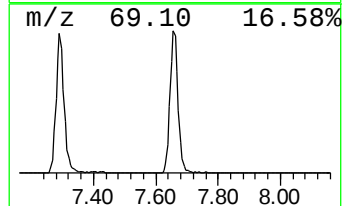
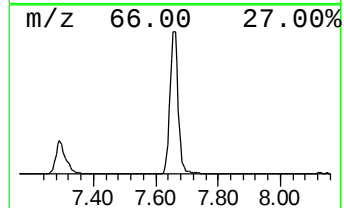
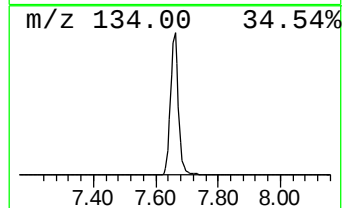
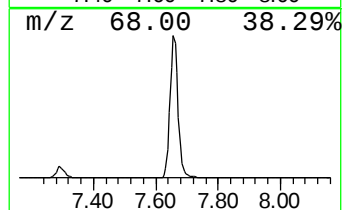
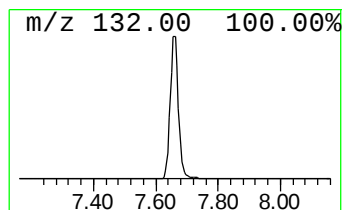
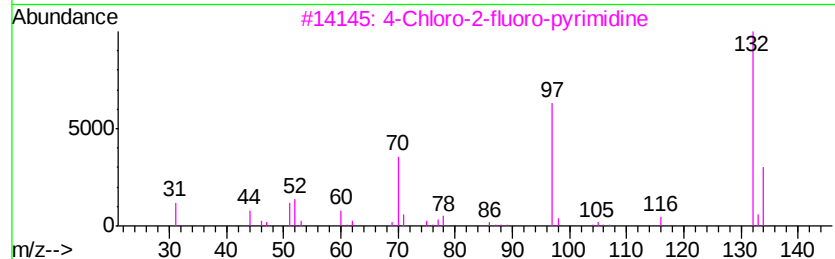
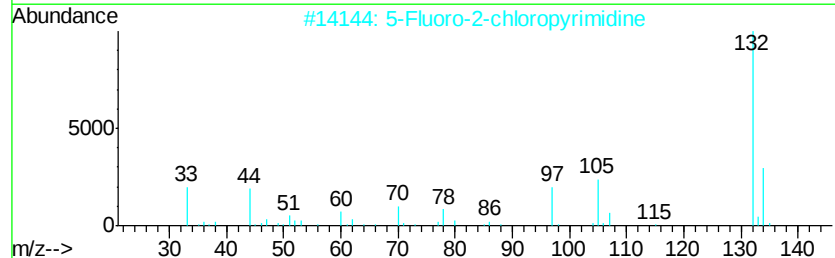
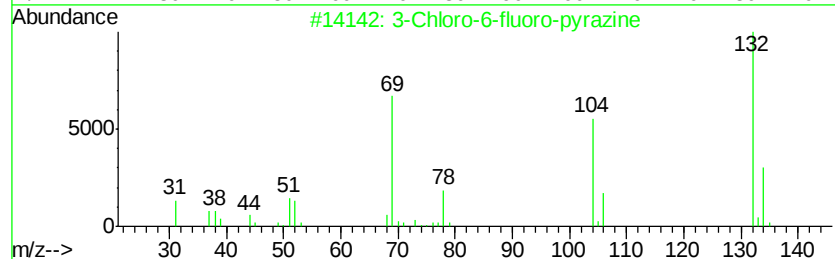
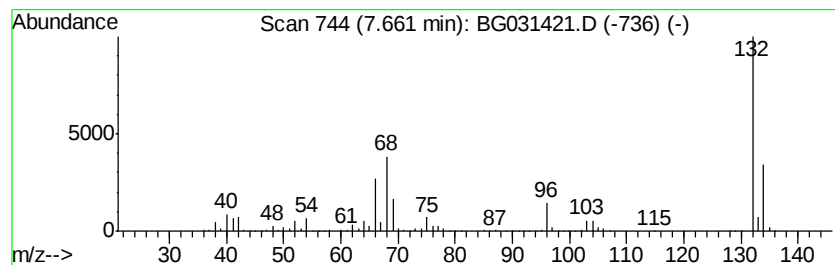
Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG111017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown7.66 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.66 | 124.01 ng | 1610620 | 1,4-Dichlorobenzene-d4 | 8.13 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |
| 5    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

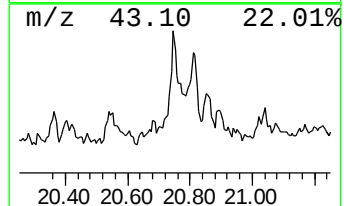
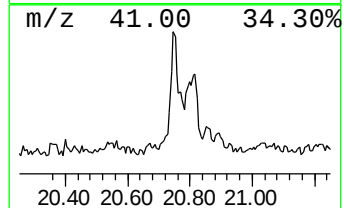
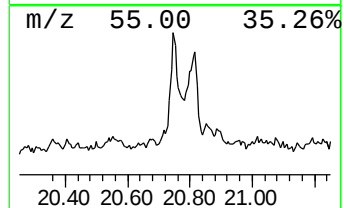
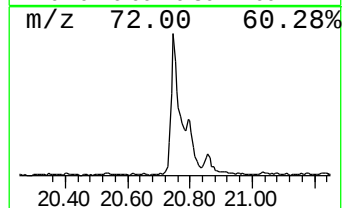
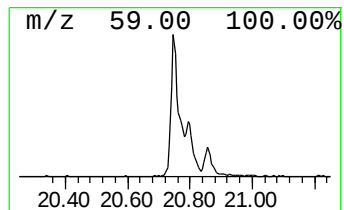
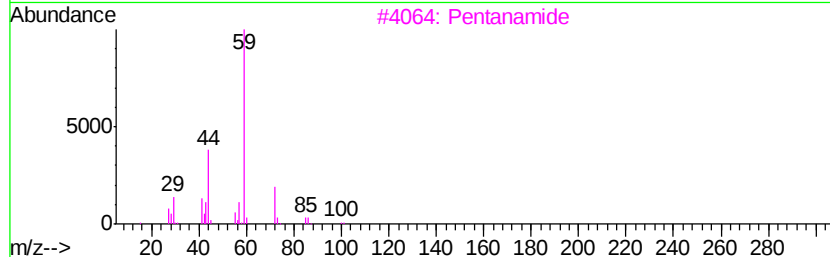
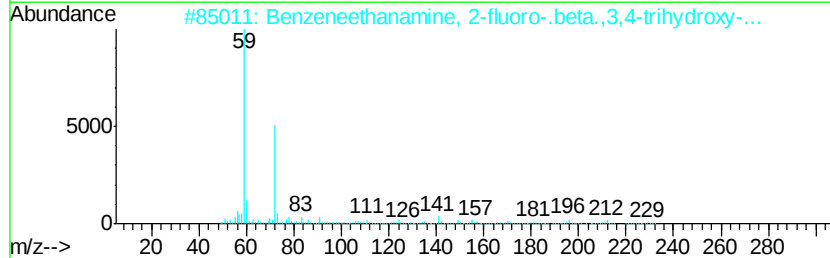
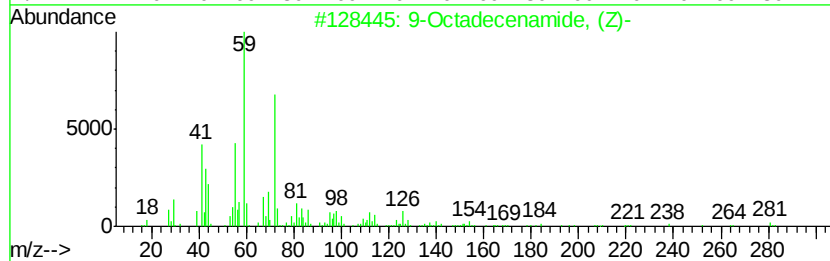
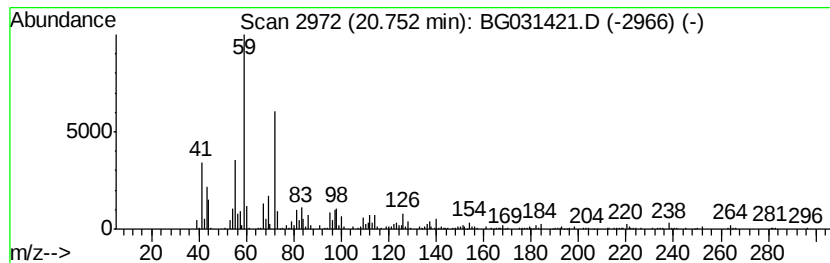
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.75 | 6.39 ng | 427727 | Chrysene-d12     | 21.76 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 91   |
| 2    |    | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FN03 | 061338-98-5 | 86   |
| 3    |    | Pentanamide                         | 101 | C5H11NO    | 000626-97-1 | 72   |
| 4    |    | Dodecanamide                        | 199 | C12H25NO   | 001120-16-7 | 64   |
| 5    |    | Octanamide                          | 143 | C8H17NO    | 000629-01-6 | 64   |



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ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG111017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

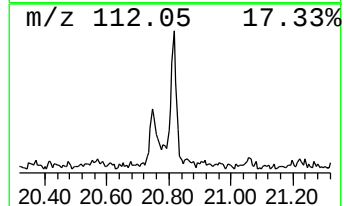
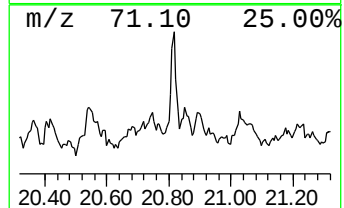
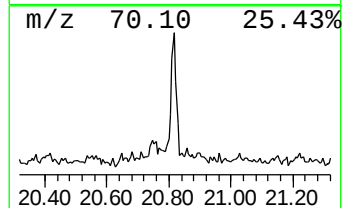
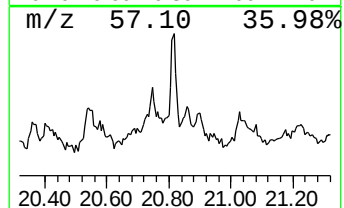
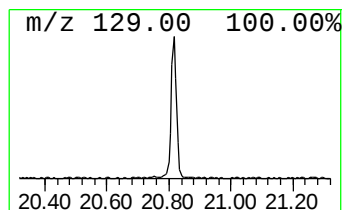
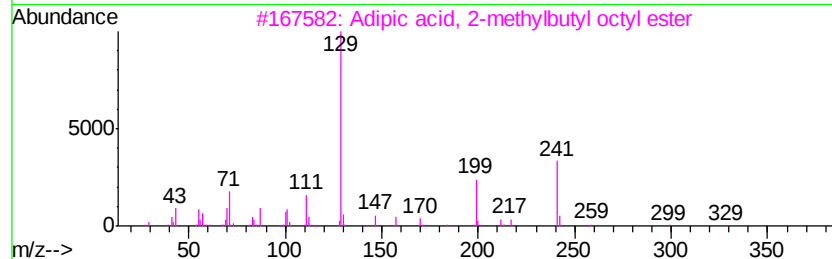
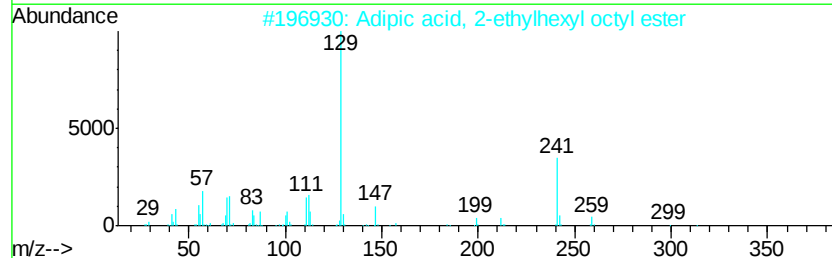
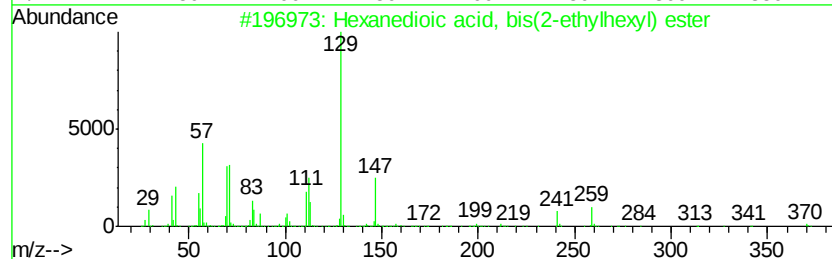
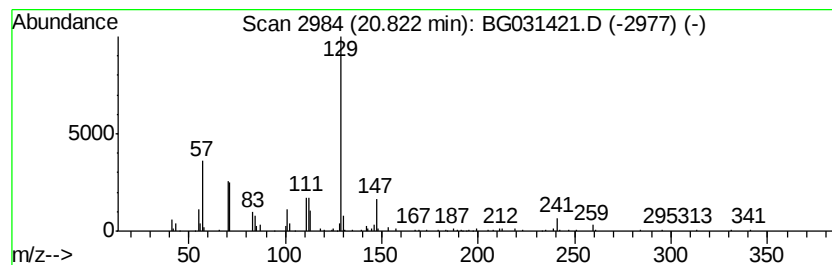
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexanedioic acid, bis(2-eth... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.82 | 5.03 ng | 336494 | Chrysene-d12     | 21.76 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Hexanedioic acid, bis(2-ethylhex... | 370 | C22H42O4 | 000103-23-1  | 91   |
| 2    |    | Adipic acid, 2-ethylhexyl octyl ... | 370 | C22H42O4 | 1000324-48-6 | 90   |
| 3    |    | Adipic acid, 2-methylbutyl octyl... | 328 | C19H36O4 | 1000324-67-7 | 59   |
| 4    |    | Adipic acid, 2-methylpent-3-yl p... | 300 | C17H32O4 | 1000353-55-9 | 47   |
| 5    |    | Adipic acid, 2-ethylhexyl isohex... | 342 | C20H38O4 | 1000324-48-3 | 43   |



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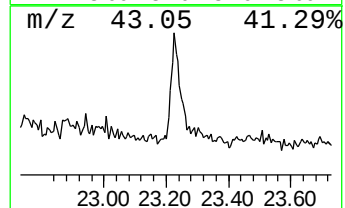
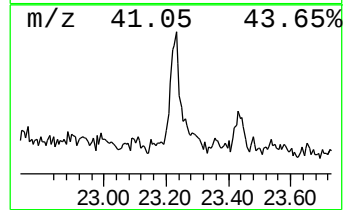
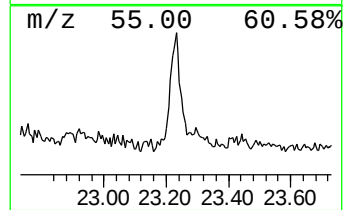
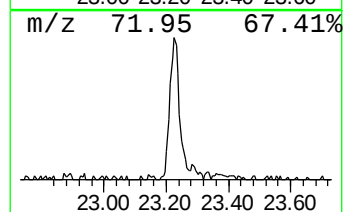
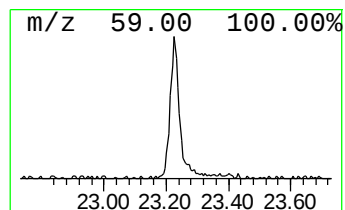
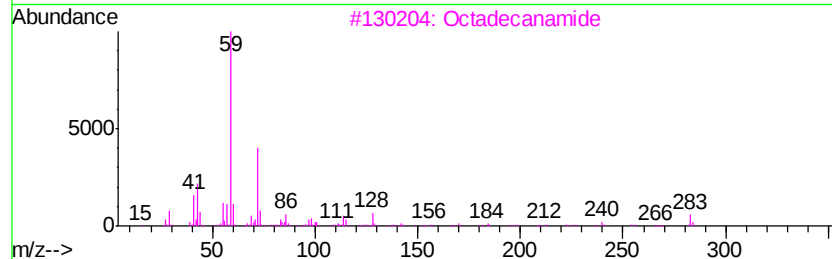
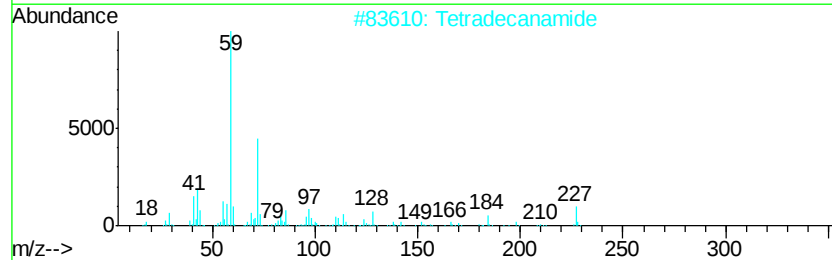
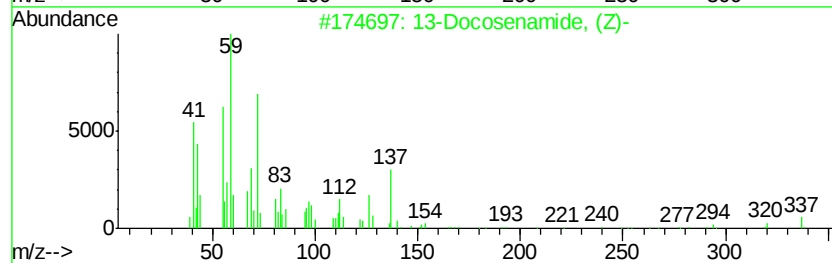
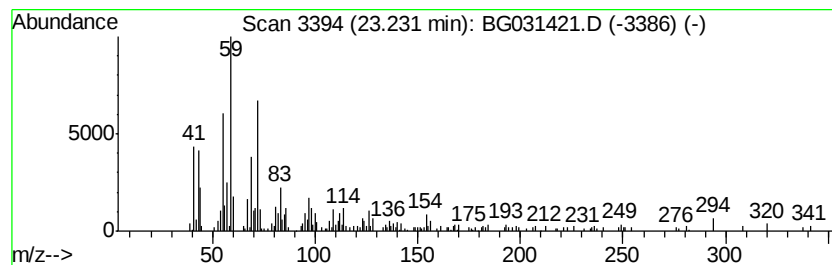
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 23.23 | 3.60 ng | 241011 | Chrysene-d12     | 21.76 |

| Hit# of | 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|---------|---|------------------------|-----|----------|-------------|------|
| 1       |   | 13-Docosenamide, (Z)-  | 337 | C22H43NO | 000112-84-5 | 87   |
| 2       |   | Tetradecanamide        | 227 | C14H29NO | 000638-58-4 | 80   |
| 3       |   | Octadecanamide         | 283 | C18H37NO | 000124-26-5 | 72   |
| 4       |   | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 72   |
| 5       |   | Decanamide-            | 171 | C10H21NO | 002319-29-1 | 64   |



Data Path : S:\HPCHEM1\BNA\_G\DATA\BG120817\  
Data File : BG031421.D  
Acq On : 8 Dec 2017 13:34  
Operator : SJ/JU  
Sample : I6717-04  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
PB-3(10-20)

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG111017.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 |
| 2-Pentanone, 4-hy...  | 5.20  | 6.9     | ng    | 89747    | 1                     | 8.13  | 259762  | 20.0 |
| unknown7.66           | 7.66  | 124.0   | ng    | 1610620  | 1                     | 8.13  | 259762  | 20.0 |
| 9-Octadecenamide, ... | 20.75 | 6.4     | ng    | 427727   | 5                     | 21.76 | 1339210 | 20.0 |
| Hexanedioic acid, ... | 20.82 | 5.0     | ng    | 336494   | 5                     | 21.76 | 1339210 | 20.0 |
| 13-Docosenamide, ...  | 23.23 | 3.6     | ng    | 241011   | 5                     | 21.76 | 1339210 | 20.0 |