

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
 Data File : BG025499.D  
 Acq On : 13 Jan 2017 2:15  
 Operator : UM/SJ  
 Sample : I1125-06  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 W-32

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-BG122116.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         | 5.259       | 406           | 412         | 418          | rBV      | 187267         | 302978        | 3.77%           | 0.950%        |
| 2         | 5.741       | 487           | 494         | 506          | rBV      | 593378         | 1095105       | 13.63%          | 3.432%        |
| 3         | 7.363       | 762           | 770         | 783          | rBV      | 383841         | 753640        | 9.38%           | 2.362%        |
| 4         | 7.733       | 825           | 833         | 847          | rVB      | 1179623        | 2144988       | 26.70%          | 6.722%        |
| 5         | 8.203       | 906           | 913         | 920          | rBV      | 238635         | 437967        | 5.45%           | 1.373%        |
| 6         | 8.526       | 959           | 968         | 979          | rVB      | 1110705        | 2006683       | 24.98%          | 6.289%        |
| 7         | 9.384       | 1106          | 1114        | 1127         | rBV      | 935071         | 1874371       | 23.33%          | 5.874%        |
| 8         | 11.029      | 1385          | 1394        | 1403         | rBV      | 306144         | 590908        | 7.36%           | 1.852%        |
| 9         | 13.450      | 1798          | 1806        | 1820         | rVB      | 2617761        | 4264851       | 53.09%          | 13.366%       |
| 10        | 14.825      | 2033          | 2040        | 2049         | rBV      | 556859         | 895562        | 11.15%          | 2.807%        |
| 11        | 16.317      | 2287          | 2294        | 2308         | rBV      | 2569466        | 4148466       | 51.64%          | 13.001%       |
| 12        | 17.574      | 2501          | 2508        | 2519         | rBV      | 750966         | 1246745       | 15.52%          | 3.907%        |
| 13        | 18.409      | 2646          | 2650        | 2655         | rBV2     | 102438         | 146535        | 1.82%           | 0.459%        |
| 14        | 19.666      | 2860          | 2864        | 2872         | rBV6     | 80865          | 132175        | 1.65%           | 0.414%        |
| 15        | 19.789      | 2880          | 2885        | 2889         | rBV5     | 46627          | 90809         | 1.13%           | 0.285%        |
| 16        | 19.836      | 2889          | 2893        | 2898         | rVB2     | 110515         | 144785        | 1.80%           | 0.454%        |
| 17        | 20.154      | 2941          | 2947        | 2954         | rBV      | 6091392        | 8033735       | 100.00%         | 25.178%       |
| 18        | 20.912      | 3072          | 3076        | 3082         | rVB2     | 130076         | 196963        | 2.45%           | 0.617%        |
| 19        | 21.863      | 3231          | 3238        | 3249         | rVB      | 957526         | 1718127       | 21.39%          | 5.385%        |
| 20        | 25.259      | 3806          | 3816        | 3829         | rVB2     | 545681         | 1682690       | 20.95%          | 5.274%        |

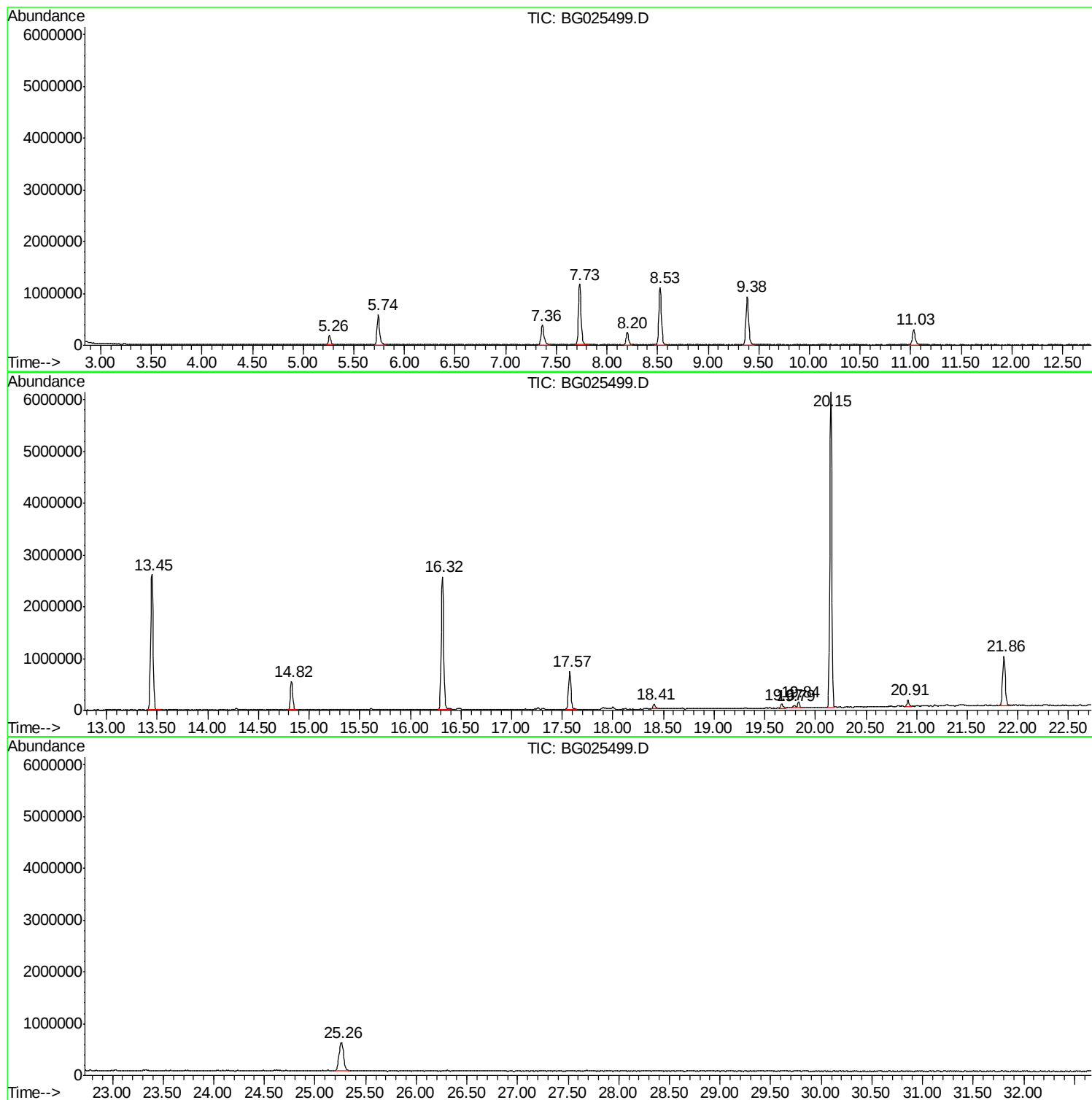
Sum of corrected areas: 31908083

Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.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\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

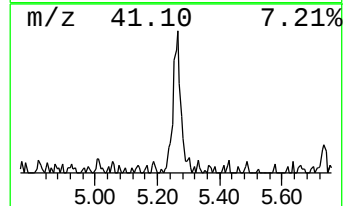
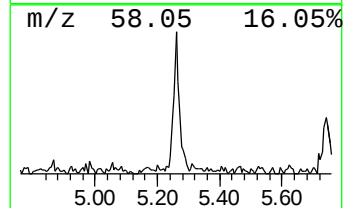
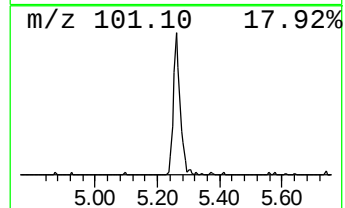
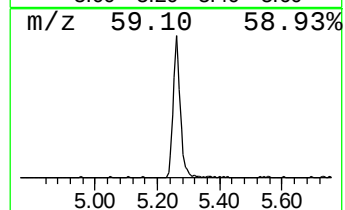
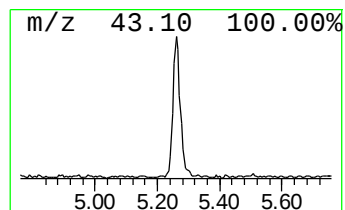
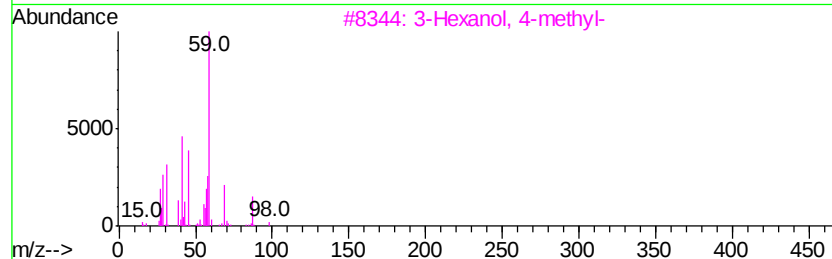
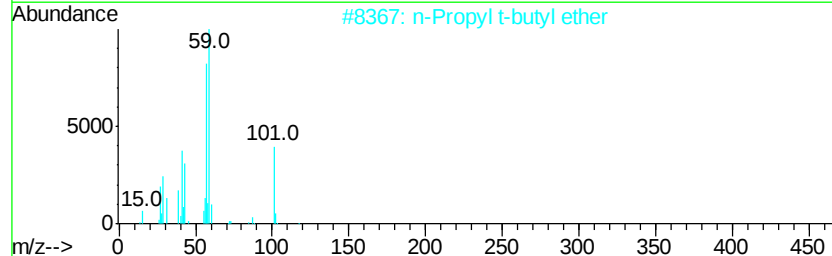
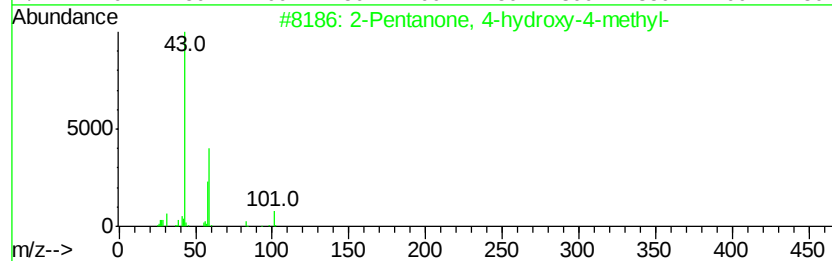
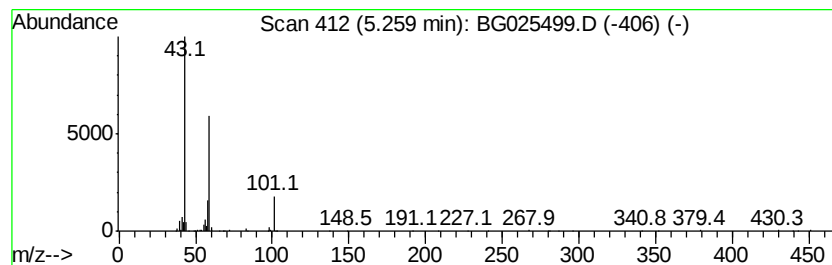
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.26 | 13.84 ng | 302978 | 1,4-Dichlorobenzene-d4 | 8.20 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#         | Qual |
|------|----|---|----------------------------------|-----|---------|--------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2  | 36   |
| 2    |    |   | n-Propyl t-butyl ether           | 116 | C7H16O  | 1000334-81-9 | 25   |
| 3    |    |   | 3-Hexanol, 4-methyl-             | 116 | C7H16O  | 000615-29-2  | 23   |
| 4    |    |   | 2,3-Butanedione, monooxime       | 101 | C4H7NO2 | 000057-71-6  | 9    |
| 5    |    |   | 3-Pentanol, 2-methyl-            | 102 | C6H14O  | 000565-67-3  | 9    |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

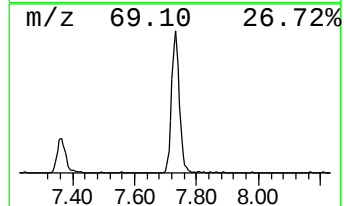
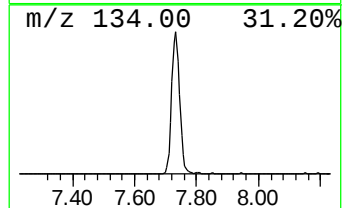
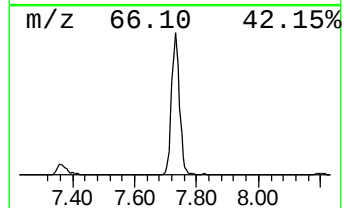
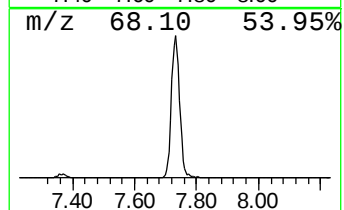
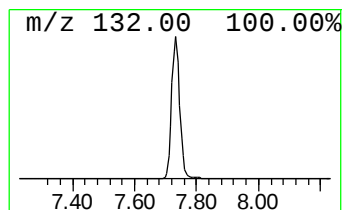
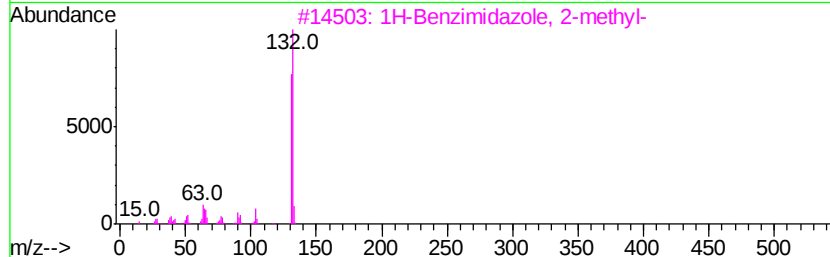
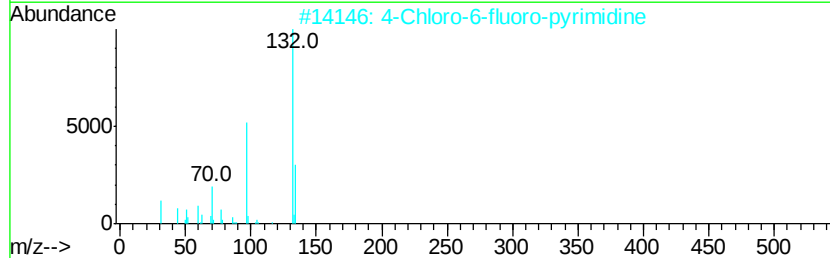
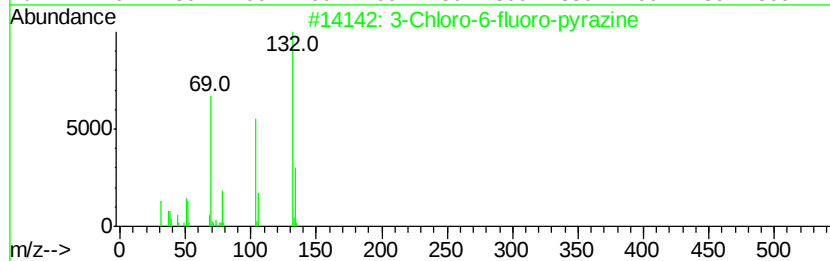
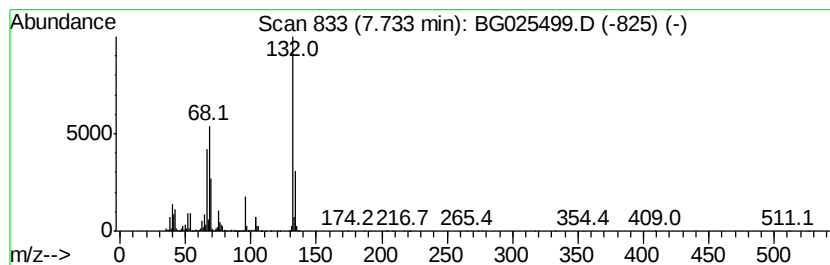
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown7.73 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.73 | 97.95 ng | 2144990 | 1,4-Dichlorobenzene-d4 | 8.20 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6  | 14   |
| 3    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6  | 10   |
| 4    |    | 3-(3,4-Dihydro-1H-isoquinolin-2-... | 377 | C24H27N03 | 1000295-80-7 | 10   |
| 5    |    | Cyclopropanamine, 1-phenyl-         | 133 | C9H11N    | 1000351-26-2 | 10   |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

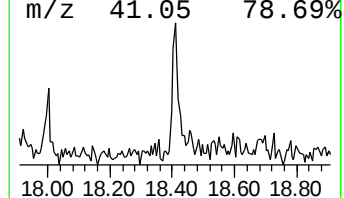
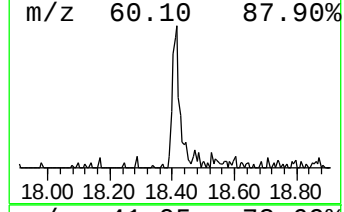
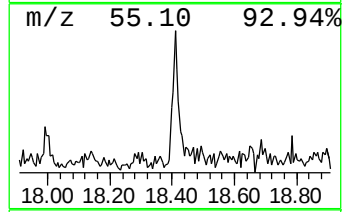
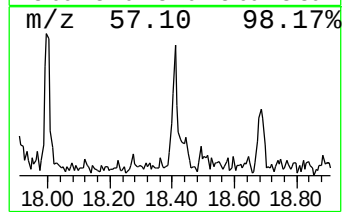
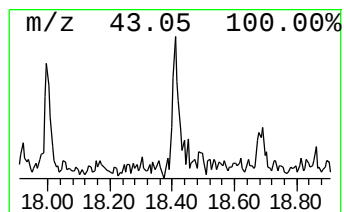
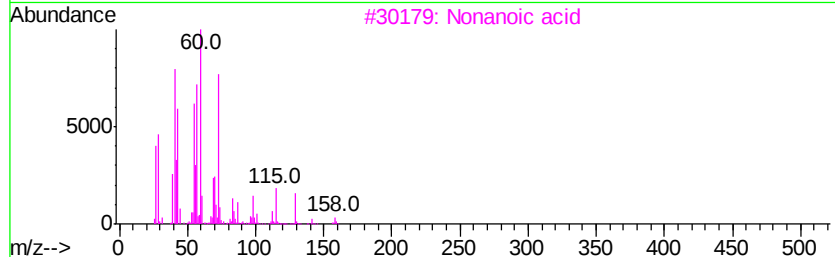
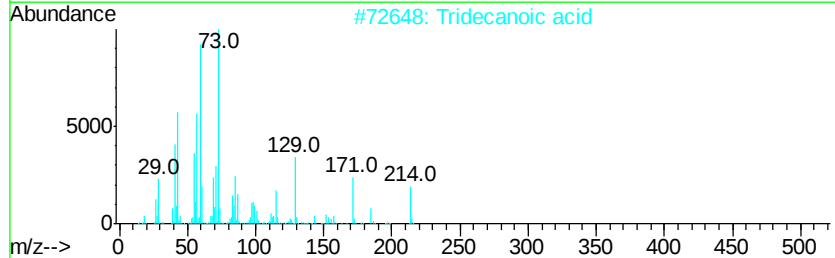
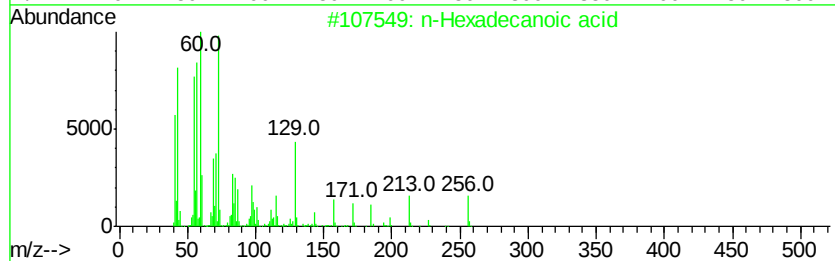
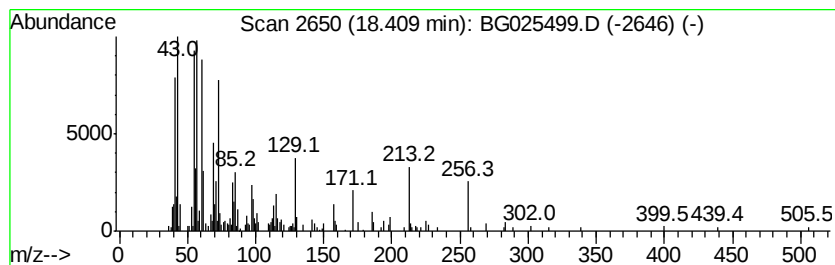
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.41 | 2.35 ng | 146535 | Phenanthrene-d10 | 17.57 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 93   |
| 2    |    | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9 | 50   |
| 3    |    | Nonanoic acid                       | 158 | C9H18O2  | 000112-05-0 | 50   |
| 4    |    | Undecanoic acid                     | 186 | C11H22O2 | 000112-37-8 | 47   |
| 5    |    | .alpha.-D-Galactopyranoside, methyl | 194 | C7H14O6  | 003396-99-4 | 38   |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

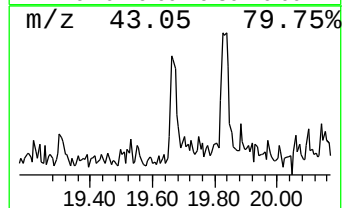
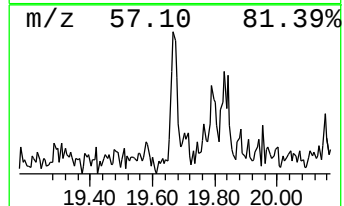
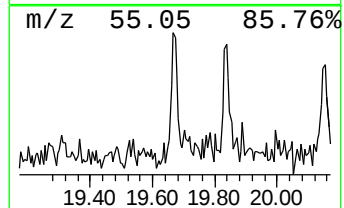
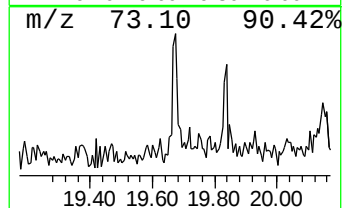
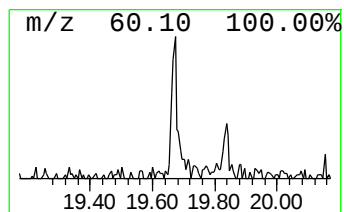
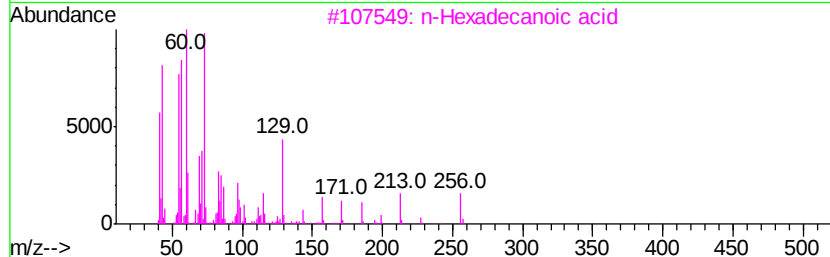
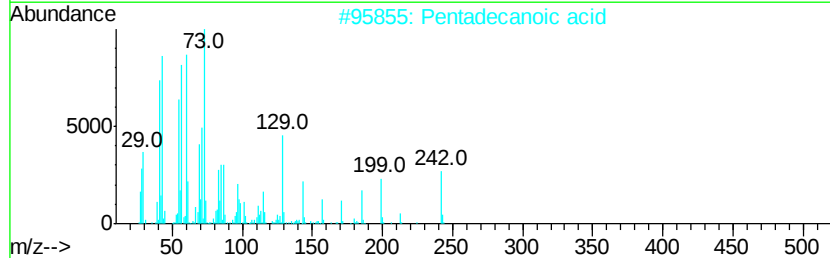
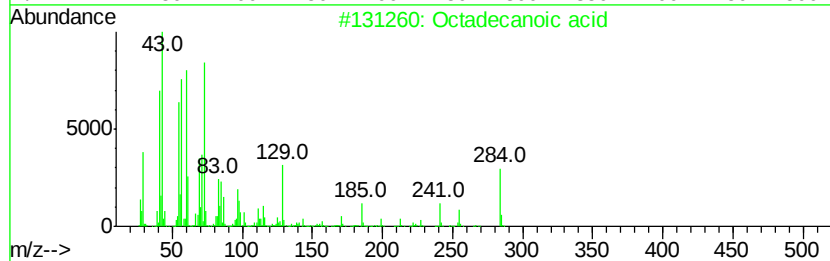
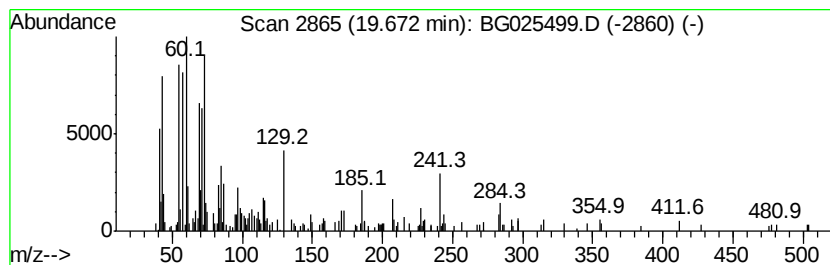
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Octadecanoic acid Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 19.67 | 2.12 ng | 132175 | Phenanthrene-d10 | 17.57 |

| Hit# of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|-----------|---------------------|-----|----------|-------------|------|
| 1         | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 89   |
| 2         | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 58   |
| 3         | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 53   |
| 4         | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 50   |
| 5         | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 50   |



Data Path : Z:\HPCHEM1\BNA G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

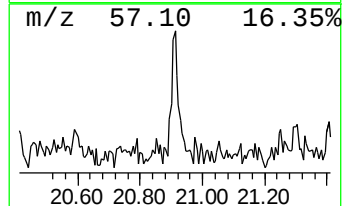
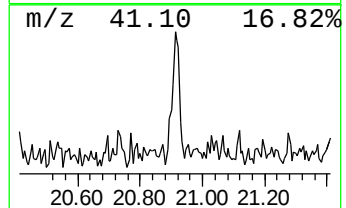
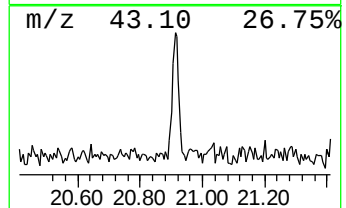
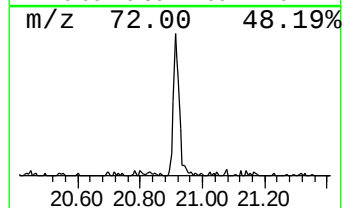
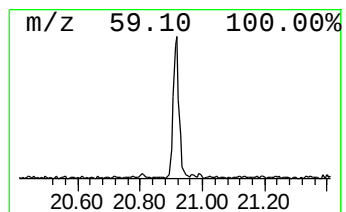
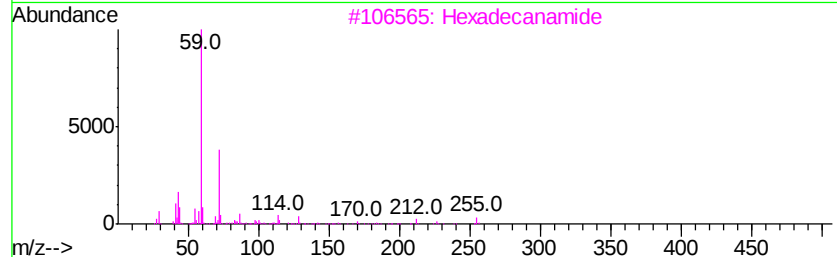
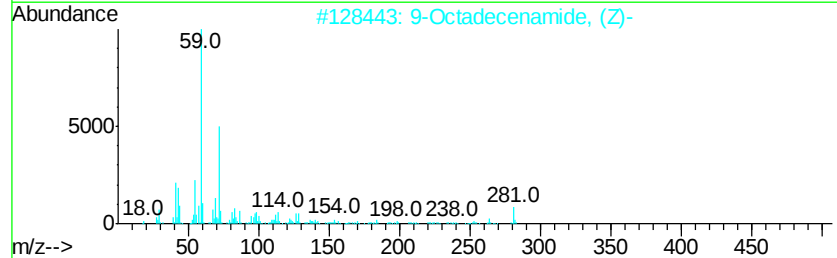
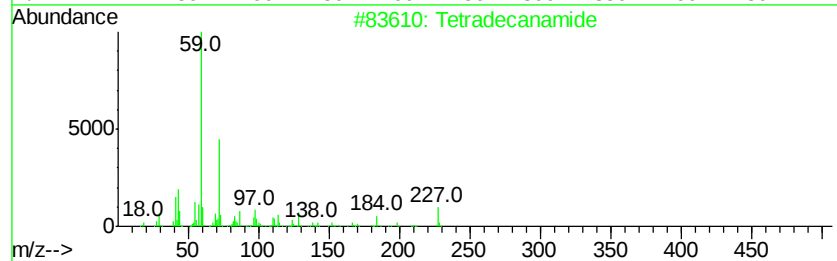
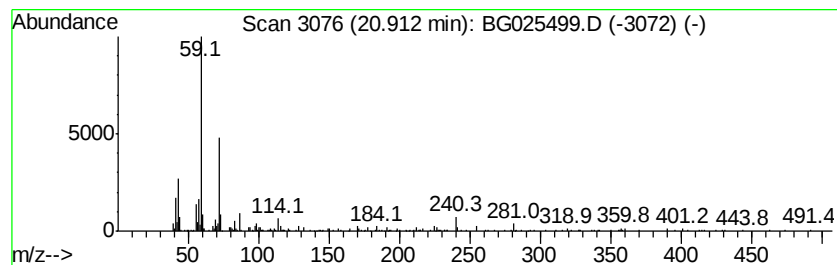
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Tetradecanamide Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.91 | 2.29 ng | 196963 | Chrysene-d12     | 21.86 |

| Hit# of | 5 | Tentative ID                   | MW  | MolForm  | CAS#        | Qual |
|---------|---|--------------------------------|-----|----------|-------------|------|
| 1       |   | Tetradecanamide                | 227 | C14H29NO | 000638-58-4 | 83   |
| 2       |   | 9-Octadecenamide, (Z)-         | 281 | C18H35NO | 000301-02-0 | 72   |
| 3       |   | Hexadecanamide                 | 255 | C16H33NO | 000629-54-9 | 72   |
| 4       |   | Heptanamide, 4-ethyl-5-methyl- | 171 | C10H21NO | 054789-40-1 | 64   |
| 5       |   | Octadecanamide                 | 283 | C18H37NO | 000124-26-5 | 56   |



Data Path : Z:\HPCHEM1\BNA\_G\DATA\BG011217\  
Data File : BG025499.D  
Acq On : 13 Jan 2017 2:15  
Operator : UM/SJ  
Sample : I1125-06  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
W-32

Quant Method : Z:\HPCHEM1\BNA\_G\METHODS\8270-BG122116.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... | 5.26  | 13.8    | ng    | 302978   | 1                     | 8.20  | 437967  | 20.0 |
| unknown7.73          | 7.73  | 98.0    | ng    | 2144990  | 1                     | 8.20  | 437967  | 20.0 |
| n-Hexadecanoic acid  | 18.41 | 2.4     | ng    | 146535   | 4                     | 17.57 | 1246750 | 20.0 |
| Octadecanoic acid    | 19.67 | 2.1     | ng    | 132175   | 4                     | 17.57 | 1246750 | 20.0 |
| Tetradecanamide      | 20.91 | 2.3     | ng    | 196963   | 5                     | 21.86 | 1718130 | 20.0 |