

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF091318\  
 Data File : BF108974.D  
 Acq On : 13 Sep 2018 19:43  
 Operator : JU/SJ  
 Sample : J4875-02  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 091118-JETT-F-D-S

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:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF090518.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         | 4.907       | 434           | 437         | 444          | rBV      | 115023         | 120766        | 2.84%           | 0.443%        |
| 2         | 5.331       | 505           | 509         | 513          | rBV      | 1435849        | 1238877       | 29.10%          | 4.539%        |
| 3         | 6.354       | 679           | 683         | 693          | rBV      | 1048954        | 866220        | 20.34%          | 3.174%        |
| 4         | 6.495       | 703           | 707         | 710          | rBV      | 2516398        | 2201036       | 51.69%          | 8.065%        |
| 5         | 6.725       | 743           | 746         | 750          | rBV      | 926489         | 835829        | 19.63%          | 3.063%        |
| 6         | 6.884       | 769           | 773         | 777          | rBV      | 3175852        | 2944695       | 69.16%          | 10.790%       |
| 7         | 7.290       | 836           | 842         | 845          | rBV      | 2628199        | 2516607       | 59.11%          | 9.221%        |
| 8         | 8.007       | 960           | 964         | 968          | rBV      | 1261133        | 1025783       | 24.09%          | 3.759%        |
| 9         | 9.089       | 1143          | 1148        | 1151         | rBV      | 4628376        | 4257747       | 100.00%         | 15.601%       |
| 10        | 9.478       | 1210          | 1214        | 1217         | rBV      | 560586         | 439908        | 10.33%          | 1.612%        |
| 11        | 9.760       | 1258          | 1262        | 1265         | rBV      | 1301183        | 1123510       | 26.39%          | 4.117%        |
| 12        | 10.436      | 1374          | 1377        | 1381         | rVB      | 79999          | 64065         | 1.50%           | 0.235%        |
| 13        | 10.542      | 1391          | 1395        | 1398         | rBV      | 1924582        | 1674482       | 39.33%          | 6.136%        |
| 14        | 11.236      | 1509          | 1513        | 1516         | rBV      | 1256657        | 1012553       | 23.78%          | 3.710%        |
| 15        | 11.772      | 1601          | 1604        | 1615         | rBV2     | 79445          | 95832         | 2.25%           | 0.351%        |
| 16        | 12.819      | 1778          | 1782        | 1786         | rBV      | 3578042        | 3683289       | 86.51%          | 13.496%       |
| 17        | 13.860      | 1955          | 1959        | 1963         | rBV      | 1114917        | 953566        | 22.40%          | 3.494%        |
| 18        | 14.354      | 2040          | 2043        | 2048         | rBV      | 58279          | 53397         | 1.25%           | 0.196%        |
| 19        | 14.648      | 2090          | 2093        | 2098         | rBV      | 92455          | 87968         | 2.07%           | 0.322%        |
| 20        | 14.718      | 2101          | 2105        | 2110         | rVB      | 381855         | 349317        | 8.20%           | 1.280%        |
| 21        | 14.966      | 2143          | 2147        | 2154         | rVB      | 103947         | 118858        | 2.79%           | 0.436%        |
| 22        | 15.271      | 2193          | 2199        | 2204         | rBV      | 896114         | 1045486       | 24.55%          | 3.831%        |
| 23        | 15.324      | 2204          | 2208        | 2215         | rVB      | 126723         | 159873        | 3.75%           | 0.586%        |
| 24        | 15.730      | 2272          | 2277        | 2284         | rBV      | 131763         | 188469        | 4.43%           | 0.691%        |
| 25        | 16.201      | 2352          | 2357        | 2363         | rVB      | 91039          | 149226        | 3.50%           | 0.547%        |
| 26        | 16.748      | 2444          | 2450        | 2458         | rBV2     | 38144          | 83902         | 1.97%           | 0.307%        |

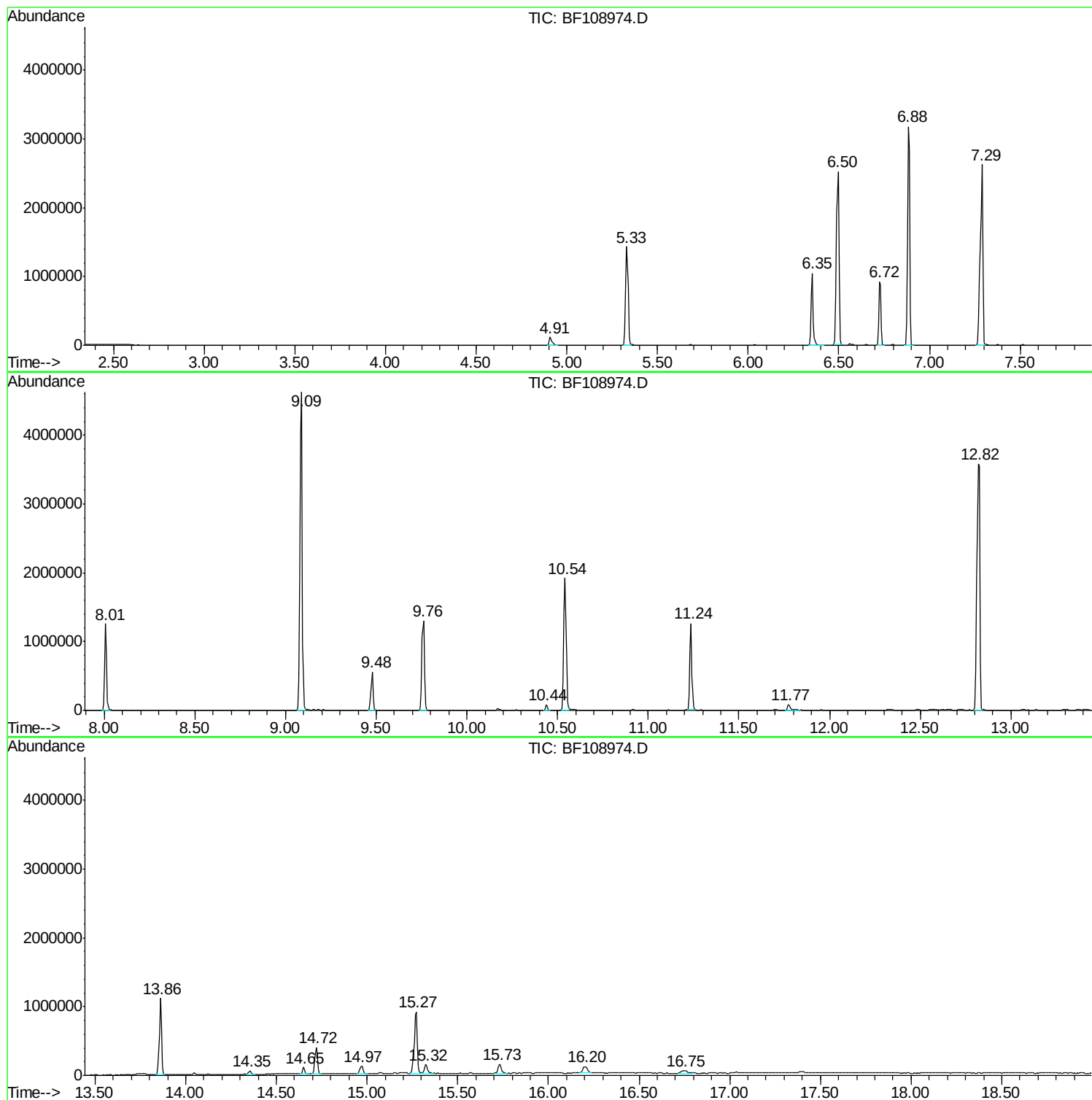
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ClientSampleId :  
091118-JETT-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.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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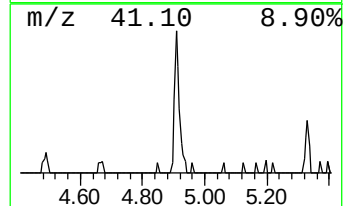
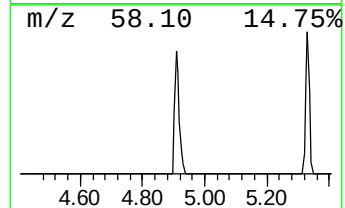
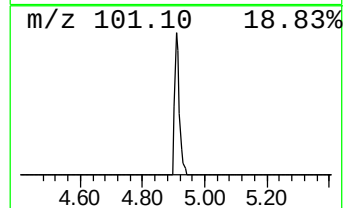
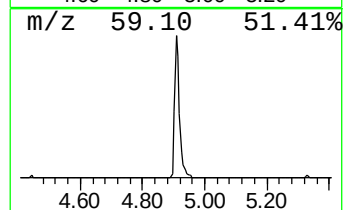
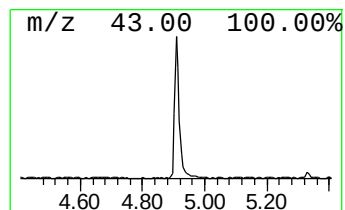
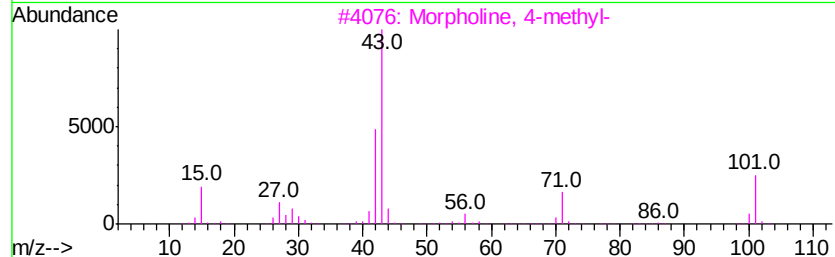
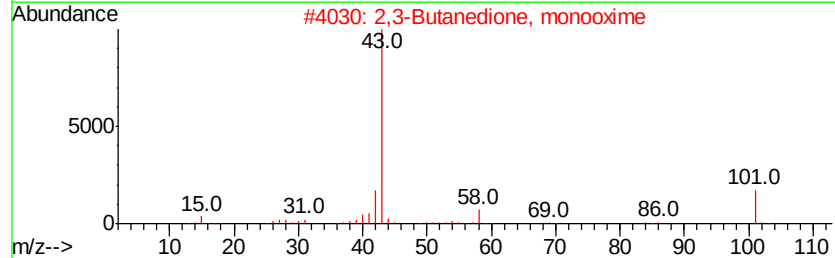
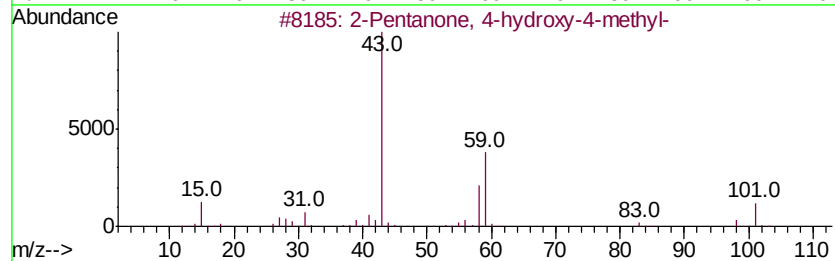
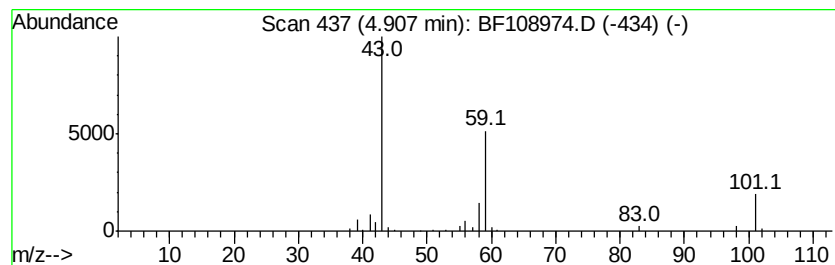
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.91 | 2.89 ng | 120766 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 56   |
| 2    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 16   |
| 3    |    | Morpholine, 4-methyl-               | 101 | C5H11NO | 000109-02-4 | 9    |
| 4    |    | 1,3-Dioxolane-2-methanol, 2,4-di... | 132 | C6H12O3 | 053951-43-2 | 9    |
| 5    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O  | 000615-29-2 | 9    |



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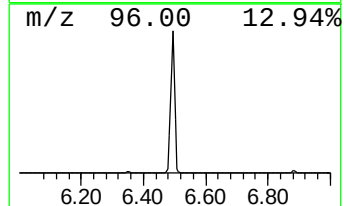
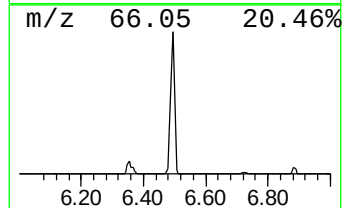
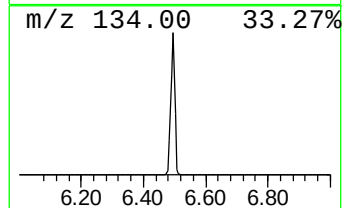
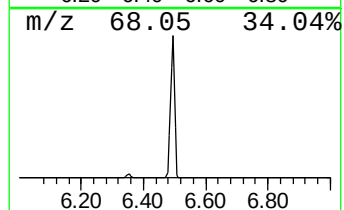
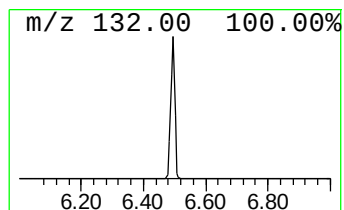
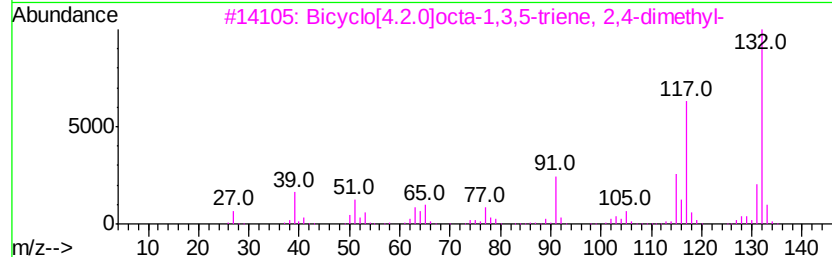
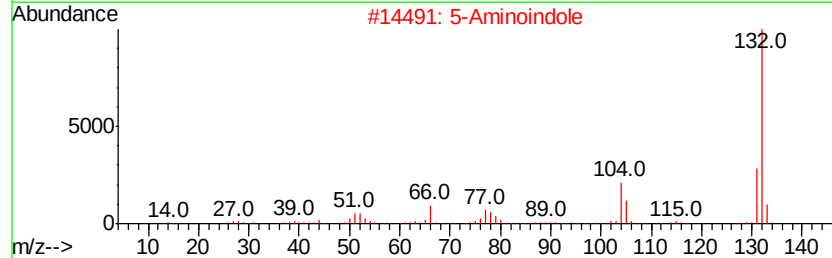
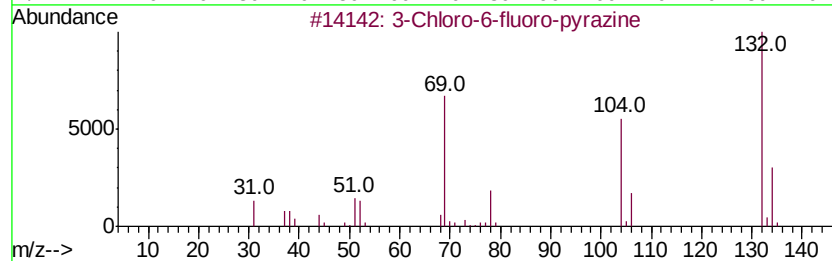
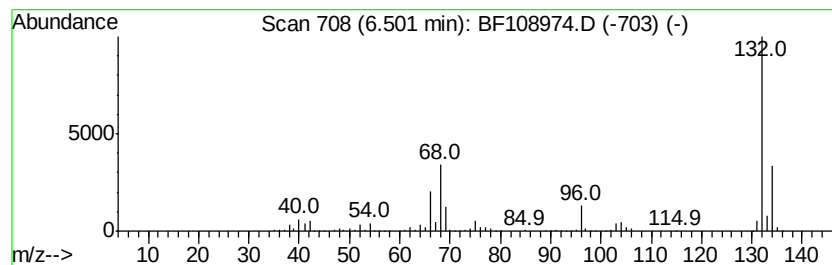
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown6.50 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.50 | 52.67 ng | 2201040 | 1,4-Dichlorobenzene-d4 | 6.73 |

| Hit# | of                                  | Tentative ID | MW        | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-----------|--------------|------|------|
| 1    | 3-Chloro-6-fluoro-pyrazine          | 132          | C4H2ClFN2 | 1000146-10-7 | 27   |      |
| 2    | 5-Aminoindole                       | 132          | C8H8N2    | 005192-03-0  | 12   |      |
| 3    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132          | C10H12    | 028749-81-7  | 9    |      |
| 4    | 4-Chloro-2-fluoro-pyrimidine        | 132          | C4H2ClFN2 | 051422-00-5  | 9    |      |
| 5    | (E)-3-Chloro-2-methyl-2-pentenal    | 132          | C6H9ClO   | 031357-76-3  | 9    |      |



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Instrument :  
 BNA\_F  
 ClientSampleId :  
 091118-JETT-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

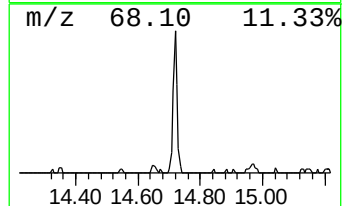
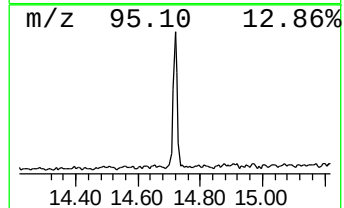
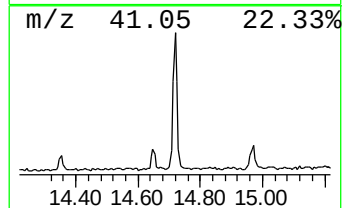
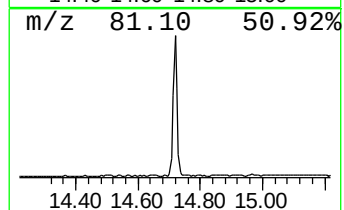
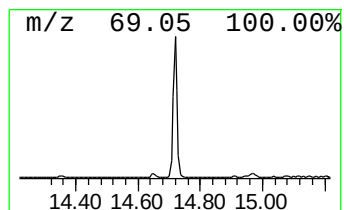
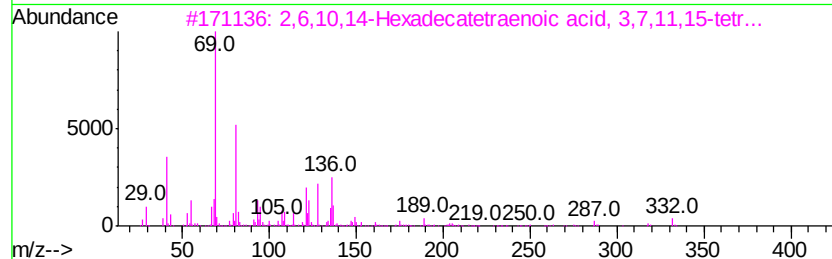
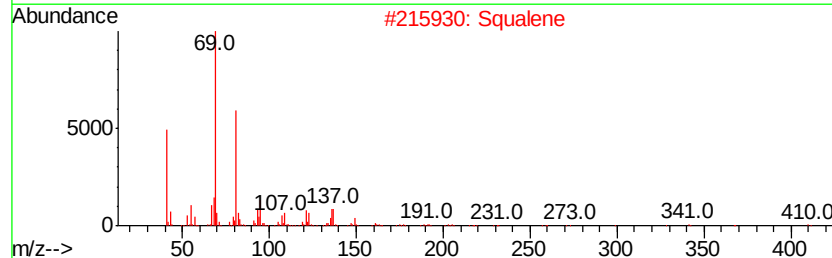
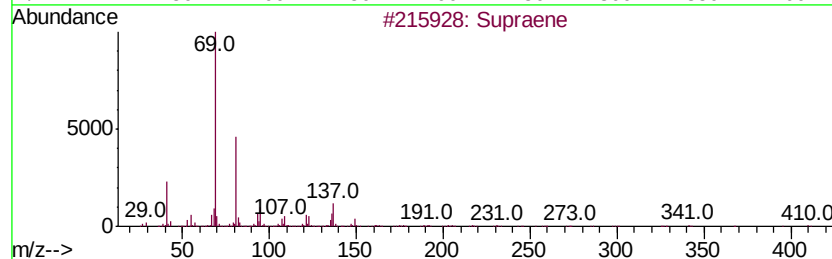
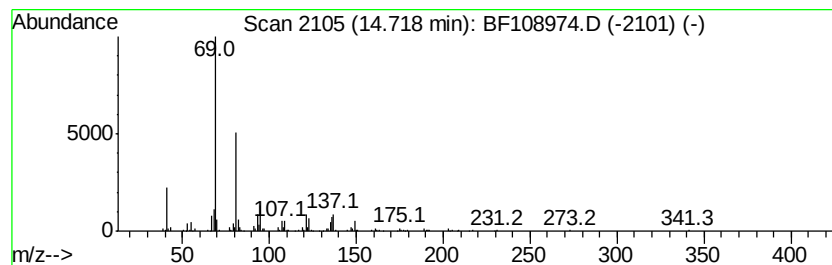
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 4 Supraene Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.72 | 6.68 ng | 349317 | Perylene-d12     | 15.27 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Supraene                            | 410 | C30H50   | 007683-64-9 | 91   |
| 2    |    | Squalene                            | 410 | C30H50   | 000111-02-4 | 91   |
| 3    |    | 2,6,10,14-Hexadecatetraenoic aci... | 332 | C22H36O2 | 024035-35-6 | 78   |
| 4    |    | 2,6,10,14-Hexadecatetraen-1-ol, ... | 332 | C22H36O2 | 061691-98-3 | 78   |
| 5    |    | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 264 | C17H28O2 | 004128-17-0 | 72   |



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091118-JETT-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF090518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

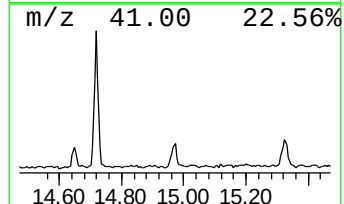
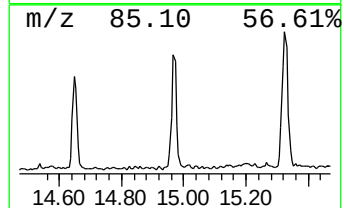
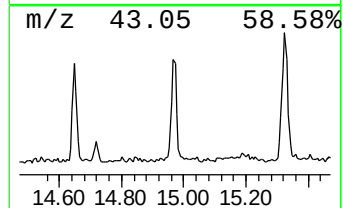
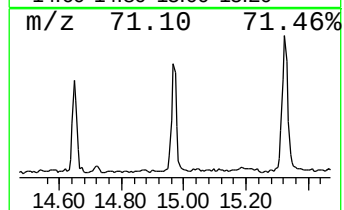
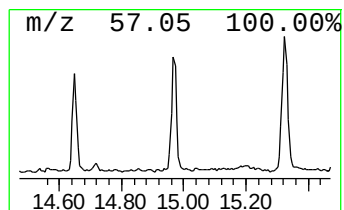
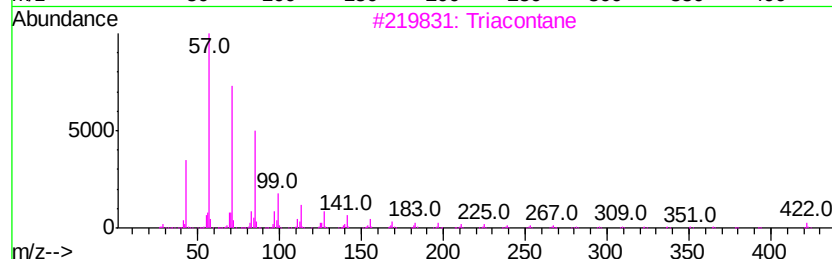
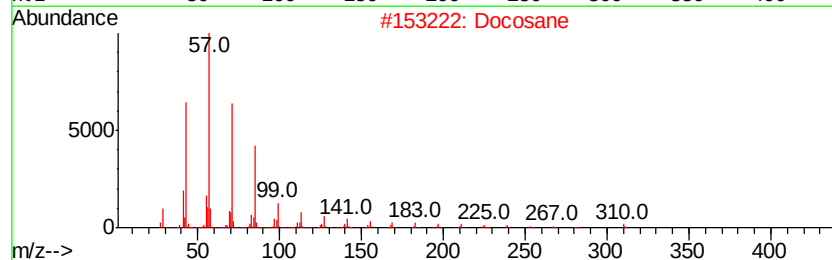
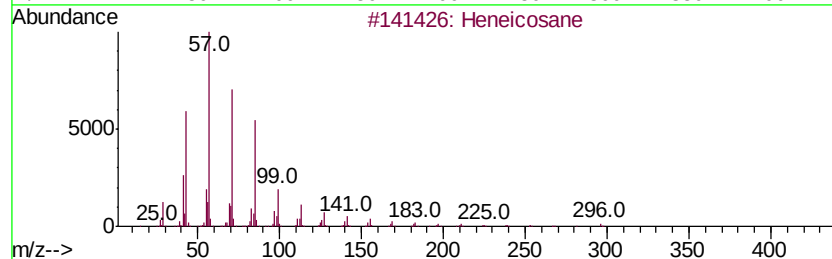
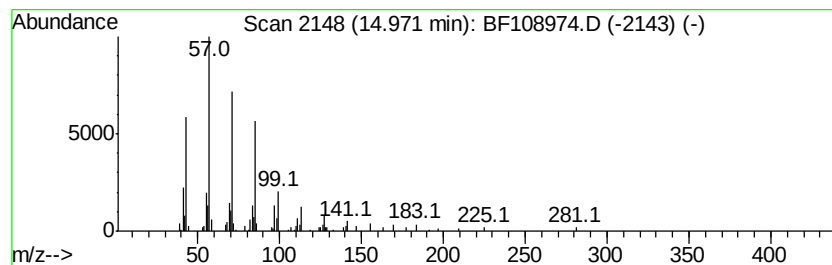
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 5 Heneicosane Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.97 | 2.27 ng | 118858 | Perylene-d12     | 15.27 |

| Hit# of | 5                   | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|---------------------|--------------|-----|---------|-------------|------|
| 1       | Heneicosane         |              | 296 | C21H44  | 000629-94-7 | 91   |
| 2       | Docosane            |              | 310 | C22H46  | 000629-97-0 | 91   |
| 3       | Triacontane         |              | 422 | C30H62  | 000638-68-6 | 91   |
| 4       | Tetracosane         |              | 338 | C24H50  | 000646-31-1 | 91   |
| 5       | Hexadecane, 1-iodo- |              | 352 | C16H33I | 000544-77-4 | 90   |



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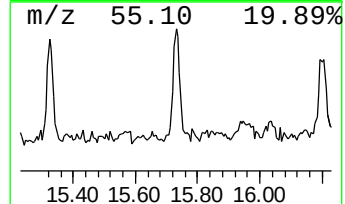
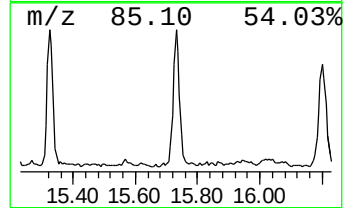
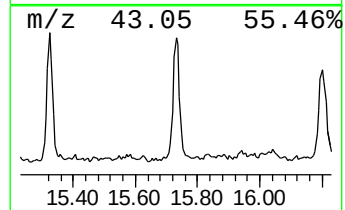
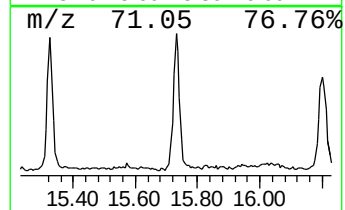
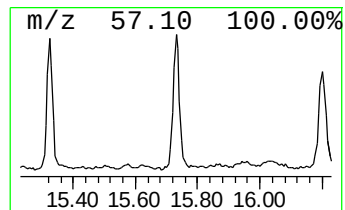
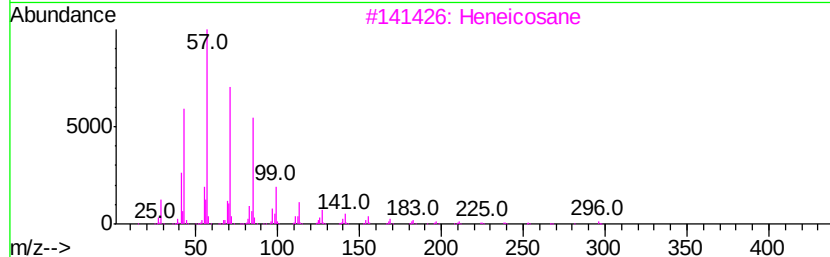
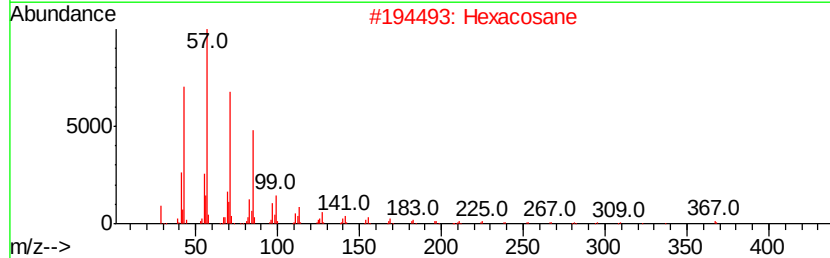
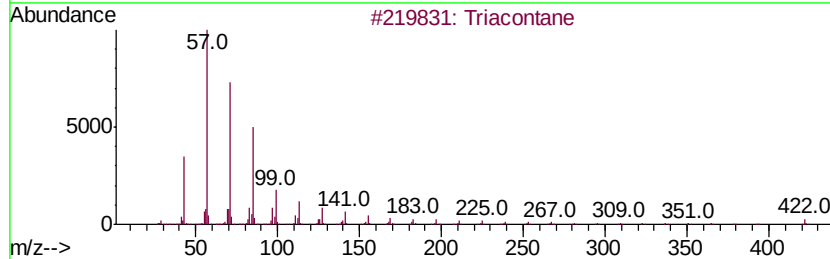
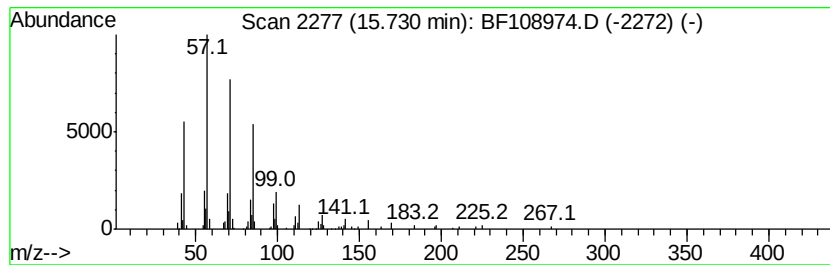
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Triacontane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.73 | 3.61 ng | 188469 | Perylene-d12     | 15.27 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|----------------------------------|-----|---------|-------------|------|
| 1    | 5  | Triacontane                      | 422 | C30H62  | 000638-68-6 | 91   |
| 2    |    | Hexacosane                       | 366 | C26H54  | 000630-01-3 | 91   |
| 3    |    | Heneicosane                      | 296 | C21H44  | 000629-94-7 | 91   |
| 4    |    | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54  | 055282-11-6 | 91   |
| 5    |    | Hexadecane, 1-iodo-              | 352 | C16H33I | 000544-77-4 | 91   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF091318\  
Data File : BF108974.D  
Acq On : 13 Sep 2018 19:43  
Operator : JU/SJ  
Sample : J4875-02  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
091118-JETT-F-D-S

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF090518.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... | 4.91  | 2.9     | ng    | 120766   | 1                     | 6.73  | 835829  | 20.0 |
| unknown6.50          | 6.50  | 52.7    | ng    | 2201040  | 1                     | 6.73  | 835829  | 20.0 |
| Supraene             | 14.72 | 6.7     | ng    | 349317   | 6                     | 15.27 | 1045490 | 20.0 |
| Heneicosane          | 14.97 | 2.3     | ng    | 118858   | 6                     | 15.27 | 1045490 | 20.0 |
| Triacontane          | 15.73 | 3.6     | ng    | 188469   | 6                     | 15.27 | 1045490 | 20.0 |