

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012018\  
 Data File : BF102265.D  
 Acq On : 20 Jan 2018 14:59  
 Operator : SJ/JU  
 Sample : J1115-15  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-37-2.0-2.5

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-BF010918.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         | 4.922       | 477           | 482         | 491          | rVB      | 175344         | 243609        | 7.19%           | 0.828%        |
| 2         | 5.334       | 546           | 552         | 555          | rBV      | 3103853        | 3233720       | 95.39%          | 10.989%       |
| 3         | 6.363       | 715           | 727         | 737          | rBV      | 3118486        | 3389897       | 100.00%         | 11.519%       |
| 4         | 6.492       | 744           | 749         | 752          | rBV      | 3303221        | 3325952       | 98.11%          | 11.302%       |
| 5         | 6.716       | 784           | 787         | 791          | rBV      | 1054462        | 881052        | 25.99%          | 2.994%        |
| 6         | 6.875       | 810           | 814         | 817          | rBV      | 2887647        | 2505106       | 73.90%          | 8.513%        |
| 7         | 7.286       | 878           | 884         | 887          | rBV      | 2225000        | 2084541       | 61.49%          | 7.084%        |
| 8         | 7.381       | 894           | 900         | 905          | rBV      | 56198          | 68679         | 2.03%           | 0.233%        |
| 9         | 7.998       | 1001          | 1005        | 1009         | rBV      | 1311628        | 1177793       | 34.74%          | 4.002%        |
| 10        | 9.080       | 1183          | 1189        | 1192         | rBV      | 3370029        | 3209199       | 94.67%          | 10.905%       |
| 11        | 9.157       | 1199          | 1202        | 1204         | rBV      | 46725          | 38938         | 1.15%           | 0.132%        |
| 12        | 9.469       | 1251          | 1255        | 1258         | rBV      | 473804         | 408515        | 12.05%          | 1.388%        |
| 13        | 9.686       | 1288          | 1292        | 1296         | rVB      | 123714         | 103289        | 3.05%           | 0.351%        |
| 14        | 9.751       | 1299          | 1303        | 1307         | rVB      | 1348280        | 1220365       | 36.00%          | 4.147%        |
| 15        | 10.157      | 1369          | 1372        | 1374         | rBV      | 73562          | 59455         | 1.75%           | 0.202%        |
| 16        | 10.186      | 1374          | 1377        | 1379         | rVB      | 123285         | 108485        | 3.20%           | 0.369%        |
| 17        | 10.404      | 1407          | 1414        | 1416         | rBV      | 41078          | 51611         | 1.52%           | 0.175%        |
| 18        | 10.545      | 1431          | 1438        | 1441         | rBV      | 1867032        | 1845609       | 54.44%          | 6.272%        |
| 19        | 10.657      | 1454          | 1457        | 1465         | rVB      | 117964         | 132026        | 3.89%           | 0.449%        |
| 20        | 11.104      | 1530          | 1533        | 1536         | rBV      | 84304          | 74220         | 2.19%           | 0.252%        |
| 21        | 11.239      | 1552          | 1556        | 1558         | rBV      | 1167334        | 1057975       | 31.21%          | 3.595%        |
| 22        | 11.527      | 1602          | 1605        | 1608         | rBV      | 62190          | 52386         | 1.55%           | 0.178%        |
| 23        | 11.633      | 1619          | 1623        | 1627         | rVB      | 39798          | 37153         | 1.10%           | 0.126%        |
| 24        | 11.933      | 1670          | 1674        | 1678         | rBV2     | 43445          | 47995         | 1.42%           | 0.163%        |
| 25        | 12.445      | 1758          | 1761        | 1765         | rVB      | 54554          | 47090         | 1.39%           | 0.160%        |
| 26        | 12.674      | 1797          | 1800        | 1802         | rBV      | 51152          | 39305         | 1.16%           | 0.134%        |
| 27        | 12.704      | 1802          | 1805        | 1815         | rVB3     | 33966          | 51911         | 1.53%           | 0.176%        |
| 28        | 12.821      | 1821          | 1825        | 1828         | rBV      | 2339722        | 2094927       | 61.80%          | 7.119%        |
| 29        | 13.715      | 1974          | 1977        | 1980         | rBV      | 167036         | 161857        | 4.77%           | 0.550%        |
| 30        | 13.874      | 1998          | 2004        | 2007         | rBV      | 791912         | 839684        | 24.77%          | 2.853%        |
| 31        | 14.351      | 2082          | 2085        | 2089         | rBV3     | 48939          | 55009         | 1.62%           | 0.187%        |
| 32        | 15.292      | 2240          | 2245        | 2254         | rVB      | 576493         | 739894        | 21.83%          | 2.514%        |
| 33        | 15.727      | 2317          | 2319        | 2323         | rVB2     | 36970          | 40416         | 1.19%           | 0.137%        |

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Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-37-2.0-2.5

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-BF010918.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

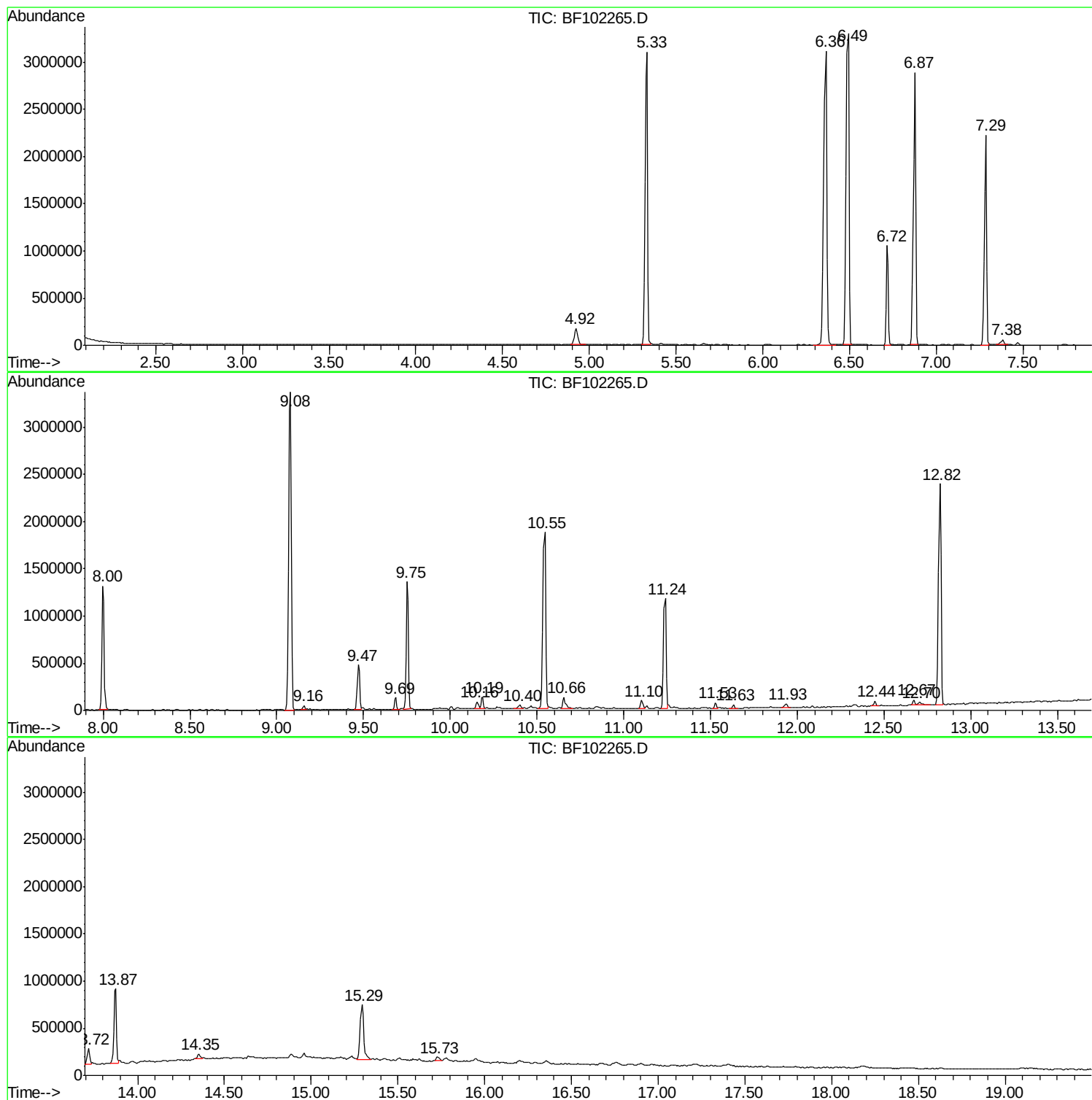
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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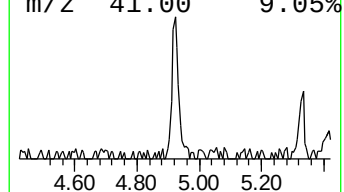
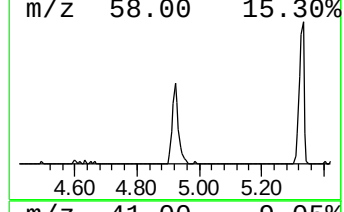
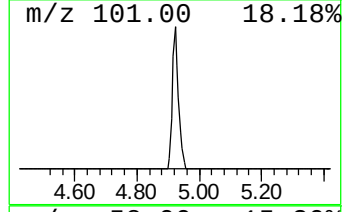
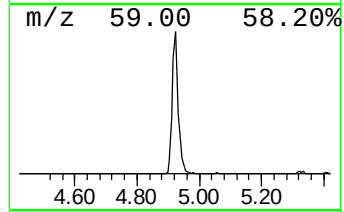
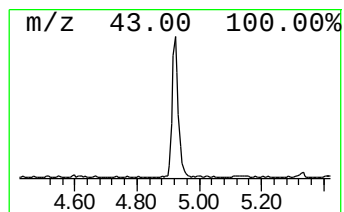
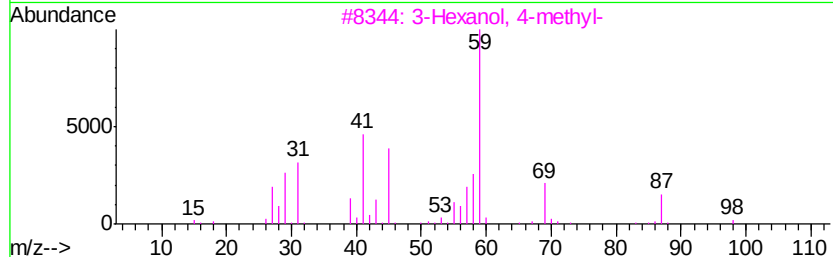
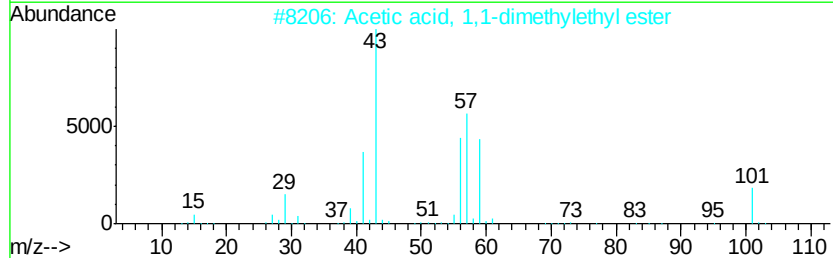
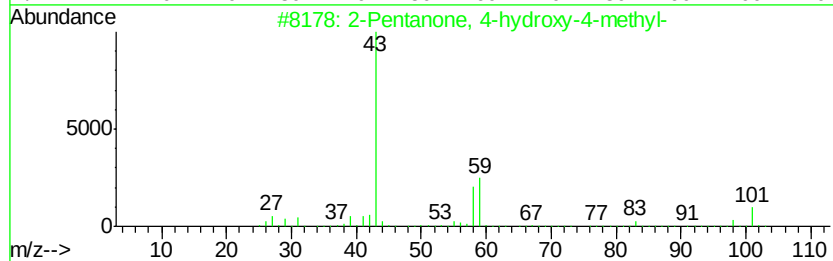
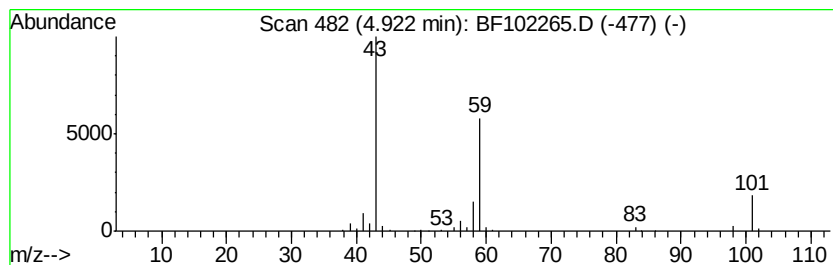
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.92 | 5.53 ng | 243609 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 59   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39   |
| 3    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O  | 000615-29-2 | 33   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 9    |
| 5    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO | 000109-02-4 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

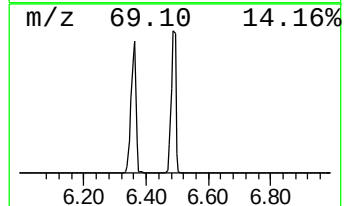
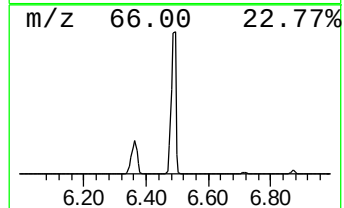
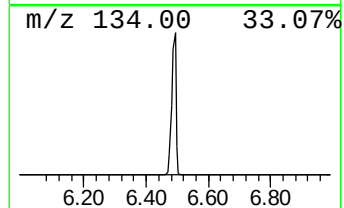
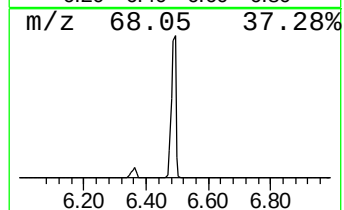
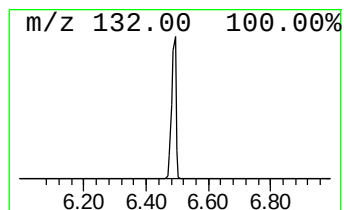
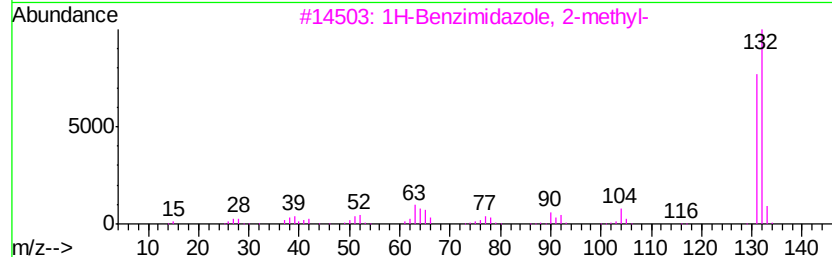
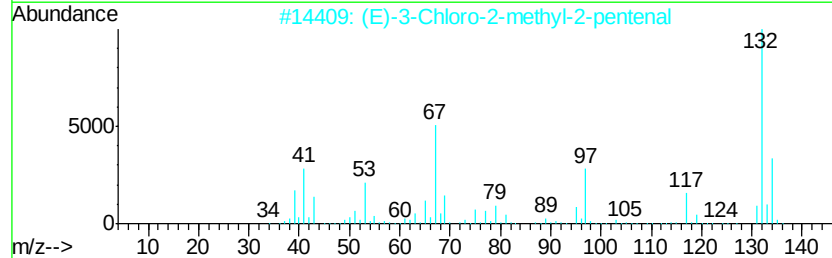
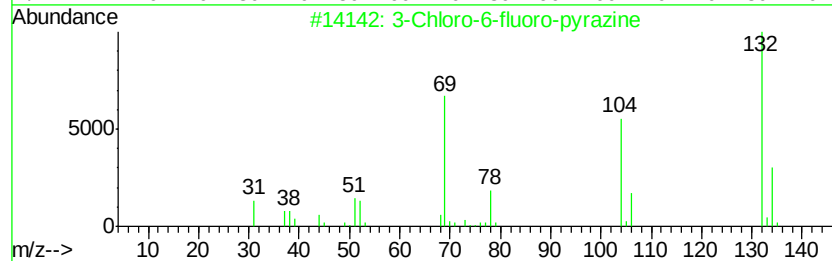
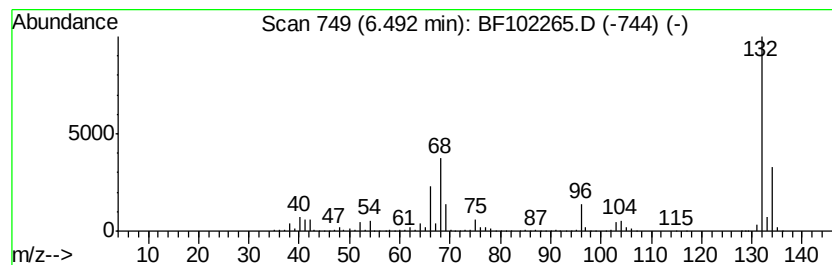
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.49 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.49 | 75.50 ng | 3325950 | 1,4-Dichlorobenzene-d4 | 6.72 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|---|----------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    |   | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    |   | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 10   |
| 4    |    |   | 1,3,5-Trifluorobenzene           | 132 | C6H3F3    | 000372-38-3  | 9    |
| 5    |    |   | (5-Methyl-2-pyridyl)acetonitrile | 132 | C8H8N2    | 1000241-93-9 | 9    |



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Misc :  
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Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF010918.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

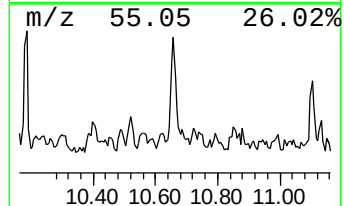
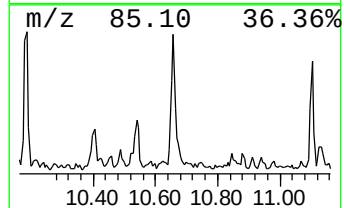
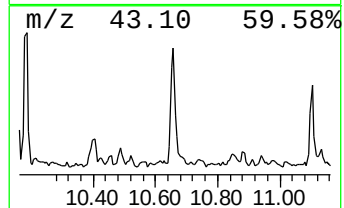
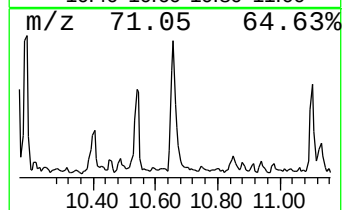
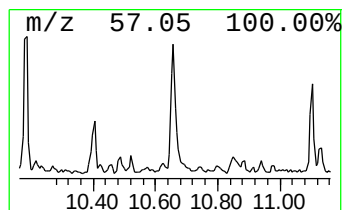
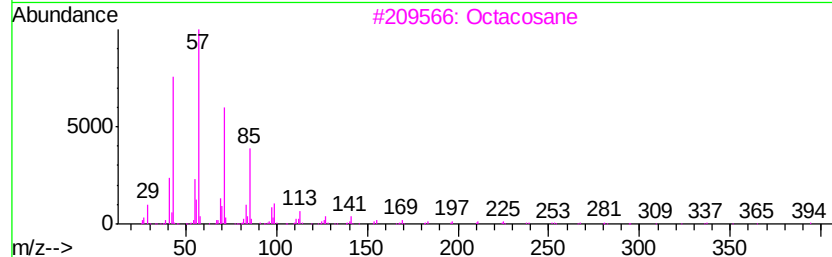
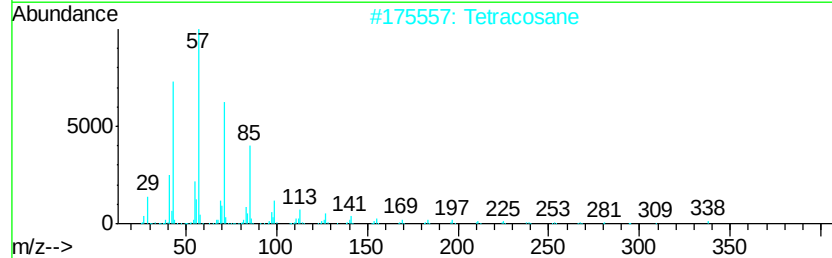
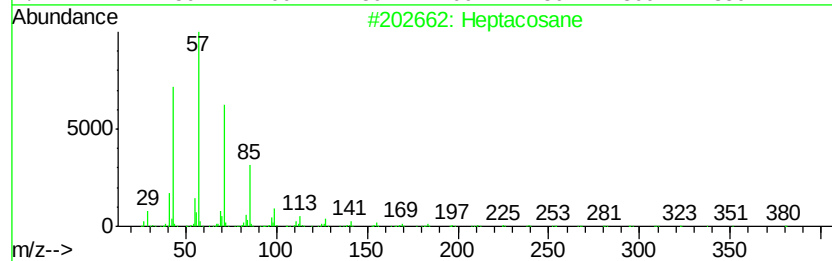
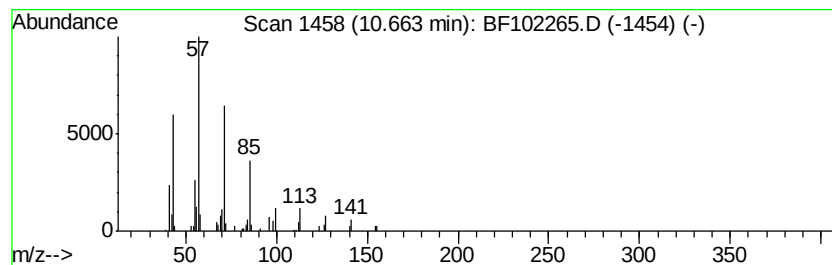
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Heptacosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 10.66 | 2.50 ng | 132026 | Phenanthrene-d10 | 11.24 |

| Hit# of | 5                            | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|------------------------------|--------------|-----|---------|-------------|------|
| 1       | Heptacosane                  |              | 380 | C27H56  | 000593-49-7 | 90   |
| 2       | Tetracosane                  |              | 338 | C24H50  | 000646-31-1 | 90   |
| 3       | Octacosane                   |              | 394 | C28H58  | 000630-02-4 | 90   |
| 4       | Dodecane, 2-methyl-6-propyl- |              | 226 | C16H34  | 055045-08-4 | 86   |
| 5       | Octadecane                   |              | 254 | C18H38  | 000593-45-3 | 86   |



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ALS Vial : 15 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF010918.M  
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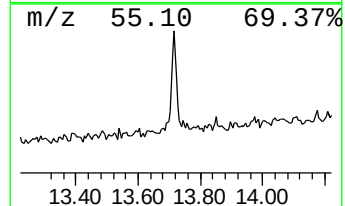
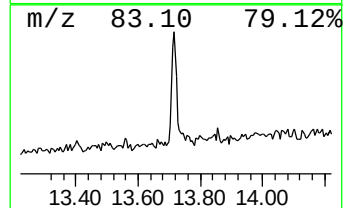
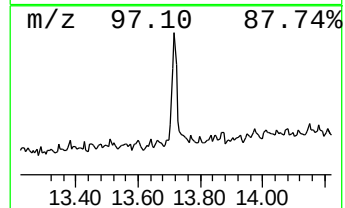
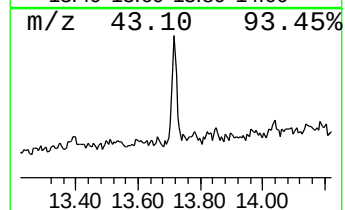
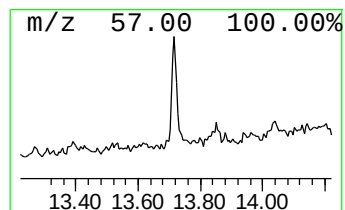
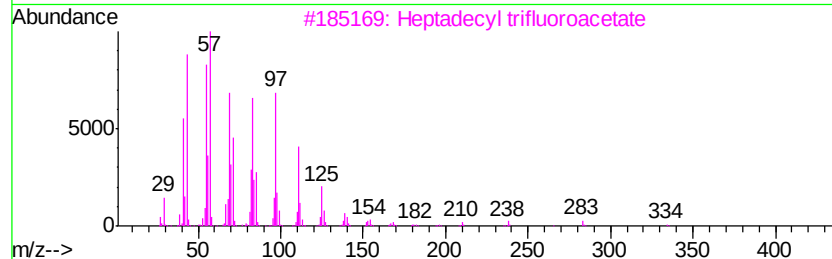
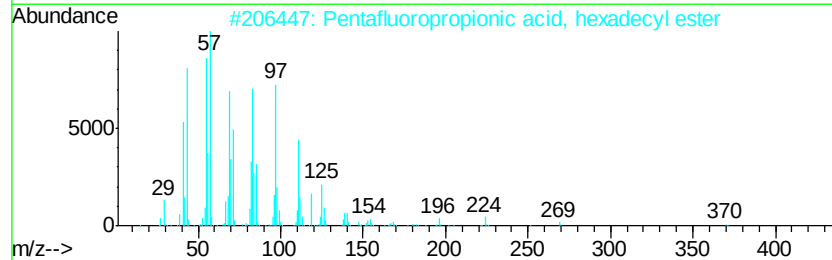
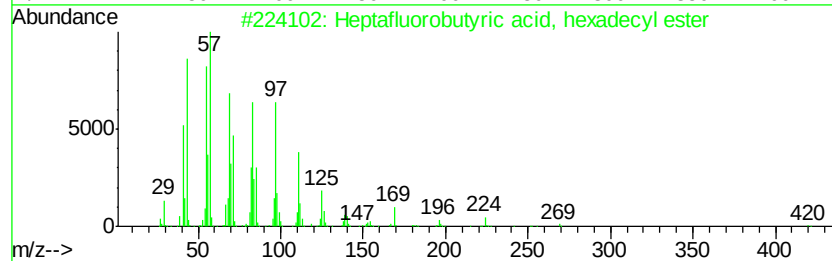
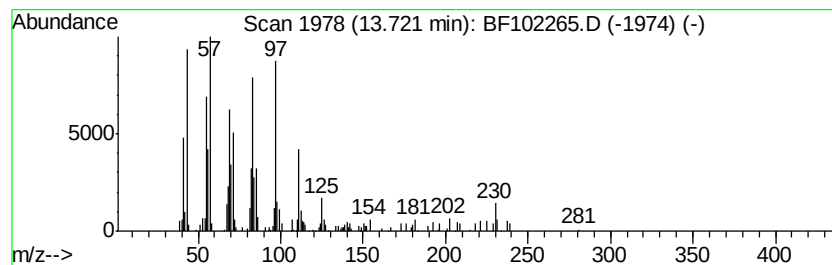
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Heptafluorobutyric acid, he... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.72 | 3.86 ng | 161857 | Chrysene-d12     | 13.87 |

| Hit# of | 5 | Tentative ID                          | MW  | MolForm    | CAS#         | Qual |
|---------|---|---------------------------------------|-----|------------|--------------|------|
| 1       |   | Heptafluorobutyric acid, hexadec...   | 438 | C20H33F7O2 | 006385-15-5  | 95   |
| 2       |   | Pentafluoropropionic acid, hexadec... | 388 | C19H33F5O2 | 006222-07-7  | 95   |
| 3       |   | Heptadecyl trifluoroacetate           | 352 | C19H35F3O2 | 1000351-87-0 | 95   |
| 4       |   | Trifluoroacetoxy hexadecane           | 338 | C18H33F3O2 | 006222-03-3  | 95   |
| 5       |   | Pentafluoropropionic acid, penta...   | 374 | C18H31F5O2 | 959092-08-1  | 94   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.92  | 5.5     | ng    | 243609   | 1                     | 6.72  | 881052  | 20.0 |
| unknown6.49          | 6.49  | 75.5    | ng    | 3325950  | 1                     | 6.72  | 881052  | 20.0 |
| Heptacosane          | 10.66 | 2.5     | ng    | 132026   | 4                     | 11.24 | 1057980 | 20.0 |
| Heptafluorobutyri... | 13.72 | 3.9     | ng    | 161857   | 5                     | 13.87 | 839684  | 20.0 |