

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070617\  
 Data File : BF096528.D  
 Acq On : 6 Jul 2017 12:59  
 Operator : SJ/MA  
 Sample : I4053-01  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 CL-02-070317-A

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-BF070117.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         | 3.081       | 166           | 169         | 190          | rBV      | 31067          | 89856         | 2.91%           | 0.358%        |
| 2         | 4.910       | 475           | 480         | 489          | rVB      | 299690         | 435674        | 14.10%          | 1.734%        |
| 3         | 5.334       | 546           | 552         | 555          | rBV      | 2885835        | 3089691       | 100.00%         | 12.299%       |
| 4         | 6.351       | 720           | 725         | 730          | rBV      | 2500584        | 2959024       | 95.77%          | 11.779%       |
| 5         | 6.487       | 743           | 748         | 751          | rBV      | 2834273        | 2859165       | 92.54%          | 11.381%       |
| 6         | 6.710       | 783           | 786         | 790          | rBV      | 919547         | 796113        | 25.77%          | 3.169%        |
| 7         | 6.869       | 809           | 813         | 817          | rBV      | 2294366        | 2153090       | 69.69%          | 8.571%        |
| 8         | 7.275       | 876           | 882         | 885          | rBV      | 1868463        | 1810521       | 58.60%          | 7.207%        |
| 9         | 7.992       | 1000          | 1004        | 1008         | rBV      | 1080055        | 966126        | 31.27%          | 3.846%        |
| 10        | 9.075       | 1182          | 1188        | 1191         | rBV      | 2996598        | 2754087       | 89.14%          | 10.963%       |
| 11        | 9.463       | 1250          | 1254        | 1258         | rBV      | 490770         | 445269        | 14.41%          | 1.772%        |
| 12        | 9.751       | 1298          | 1303        | 1306         | rBV      | 1002239        | 974211        | 31.53%          | 3.878%        |
| 13        | 10.192      | 1375          | 1378        | 1381         | rVB      | 61357          | 50498         | 1.63%           | 0.201%        |
| 14        | 10.410      | 1408          | 1415        | 1418         | rBV2     | 22200          | 32596         | 1.05%           | 0.130%        |
| 15        | 10.533      | 1432          | 1436        | 1445         | rBV      | 1365062        | 1273739       | 41.23%          | 5.070%        |
| 16        | 10.663      | 1456          | 1458        | 1466         | rVB      | 72853          | 87781         | 2.84%           | 0.349%        |
| 17        | 11.116      | 1531          | 1535        | 1538         | rBV2     | 48134          | 47592         | 1.54%           | 0.189%        |
| 18        | 11.227      | 1550          | 1554        | 1557         | rBV      | 936668         | 802954        | 25.99%          | 3.196%        |
| 19        | 12.433      | 1754          | 1759        | 1762         | rBV2     | 48407          | 55851         | 1.81%           | 0.222%        |
| 20        | 12.557      | 1777          | 1780        | 1784         | rBV4     | 32386          | 35028         | 1.13%           | 0.139%        |
| 21        | 12.663      | 1793          | 1798        | 1802         | rBV      | 37755          | 50571         | 1.64%           | 0.201%        |
| 22        | 12.816      | 1819          | 1824        | 1828         | rBV      | 1935473        | 1906473       | 61.70%          | 7.589%        |
| 23        | 13.721      | 1975          | 1978        | 1984         | rVB      | 179581         | 188806        | 6.11%           | 0.752%        |
| 24        | 13.863      | 1997          | 2002        | 2005         | rBV      | 742437         | 724940        | 23.46%          | 2.886%        |
| 25        | 15.274      | 2238          | 2242        | 2245         | rVB      | 460499         | 532250        | 17.23%          | 2.119%        |

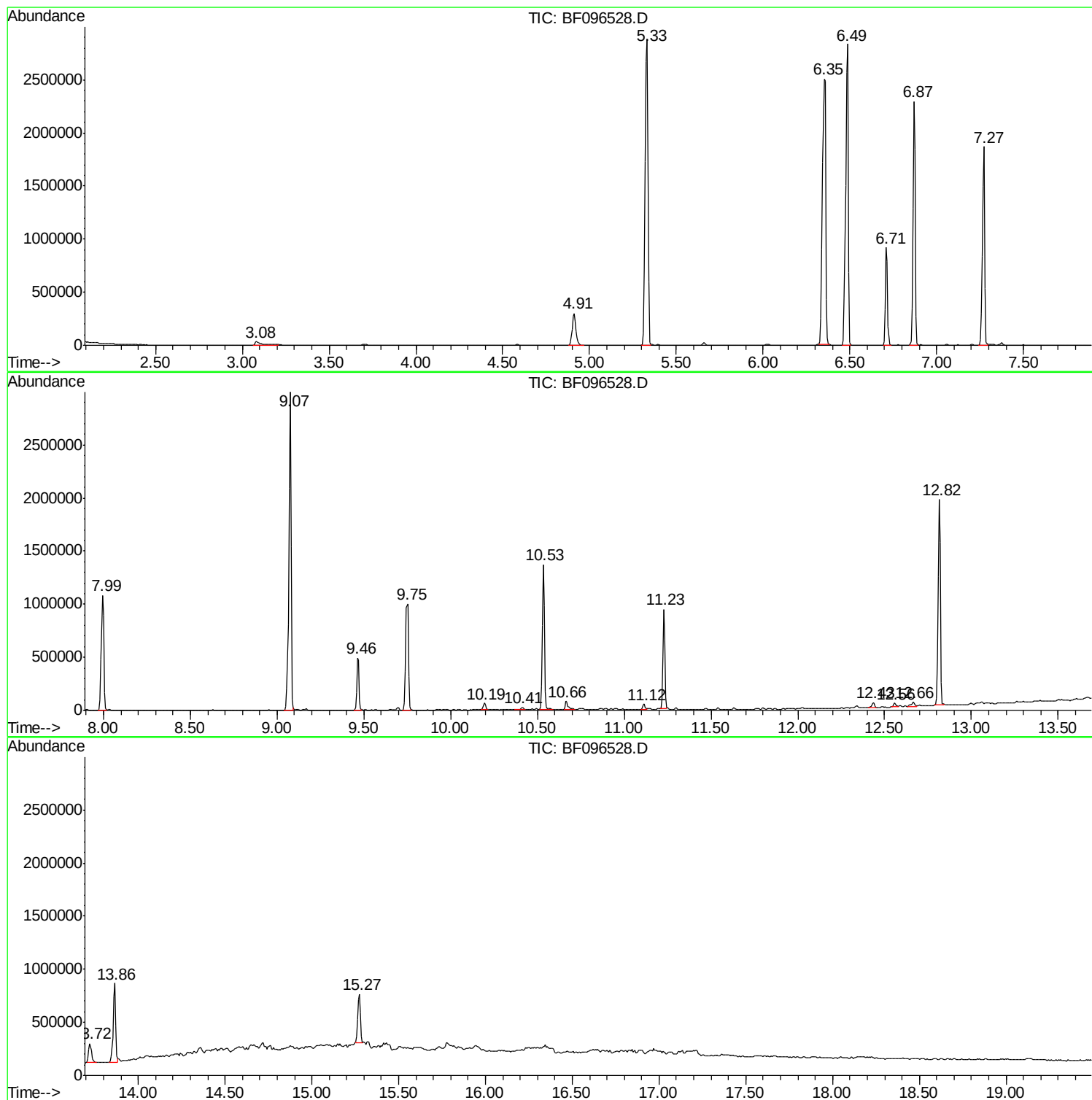
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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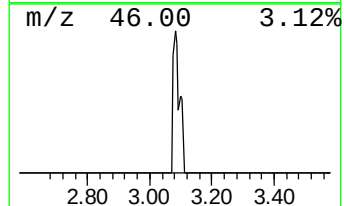
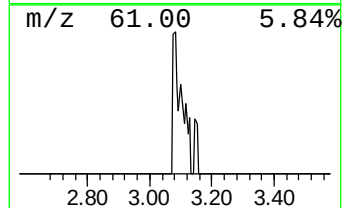
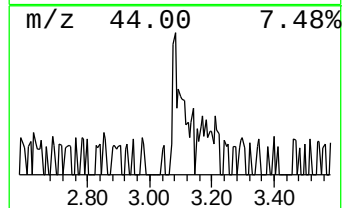
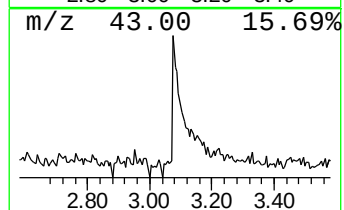
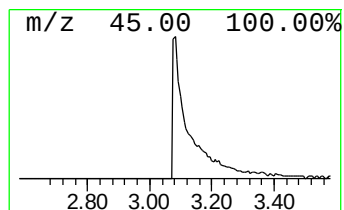
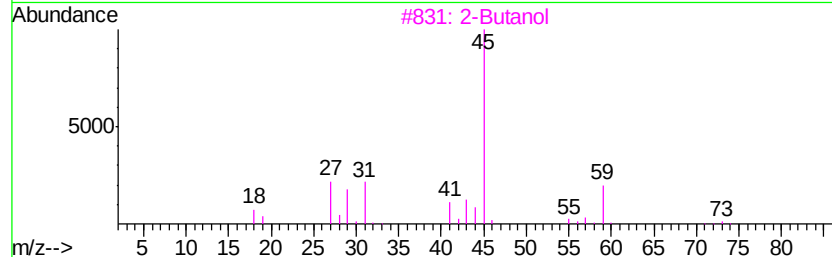
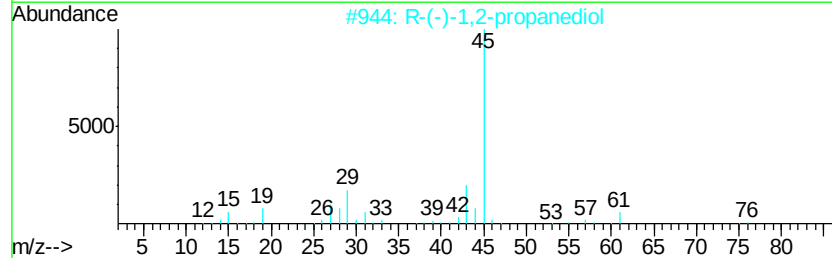
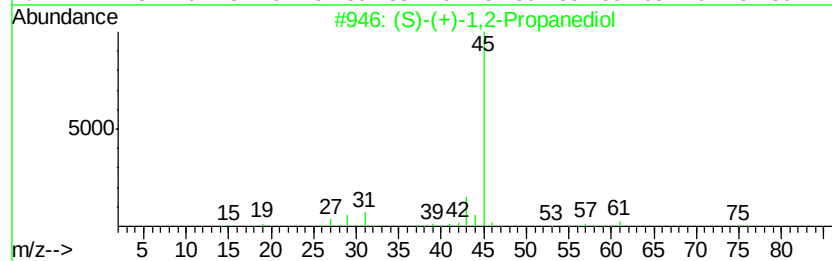
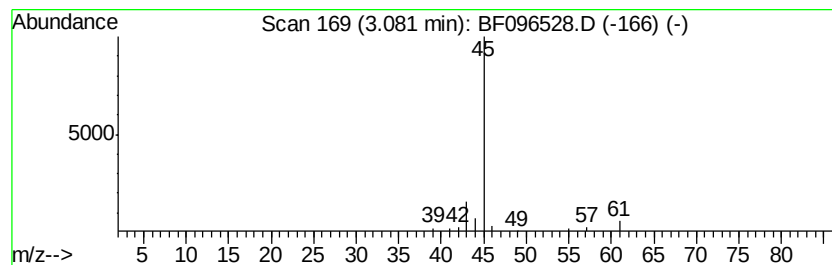
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 5

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 3.08 | 2.26 ng | 89856 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# of 5 | Tentative ID            | MW | MolForm | CAS#        | Qual |
|-----------|-------------------------|----|---------|-------------|------|
| 1         | (S)-(+)-1,2-Propanediol | 76 | C3H8O2  | 004254-15-3 | 74   |
| 2         | R-(-)-1,2-propanediol   | 76 | C3H8O2  | 004254-14-2 | 64   |
| 3         | 2-Butanol               | 74 | C4H10O  | 000078-92-2 | 43   |
| 4         | 2-Butanol, (R)-         | 74 | C4H10O  | 014898-79-4 | 43   |
| 5         | 2,3-Butanediol          | 90 | C4H10O2 | 000513-85-9 | 9    |



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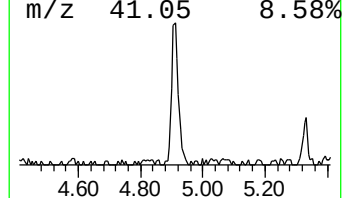
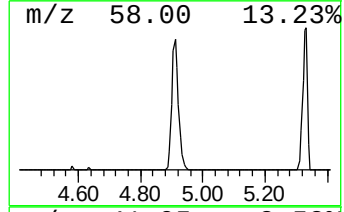
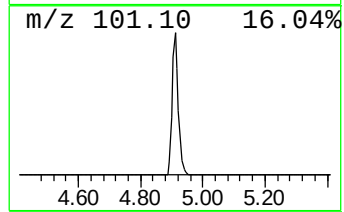
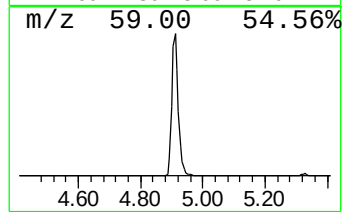
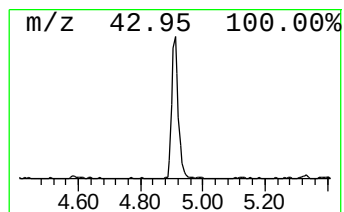
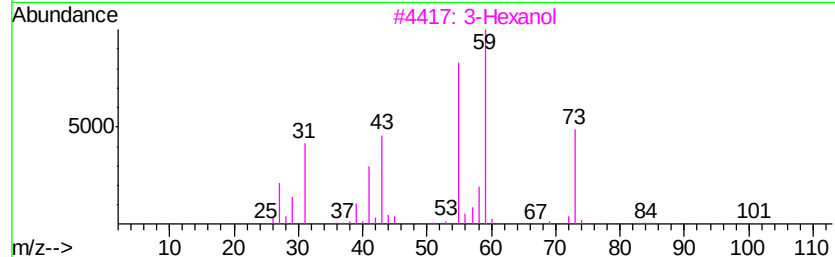
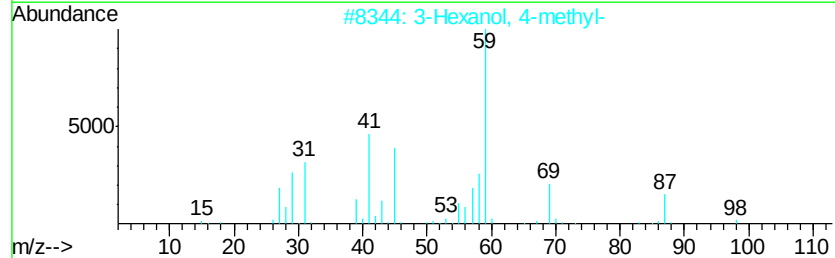
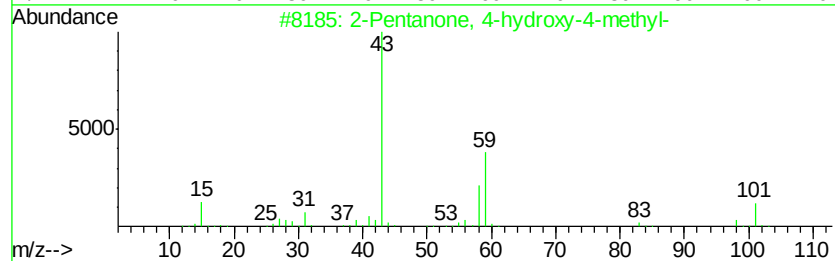
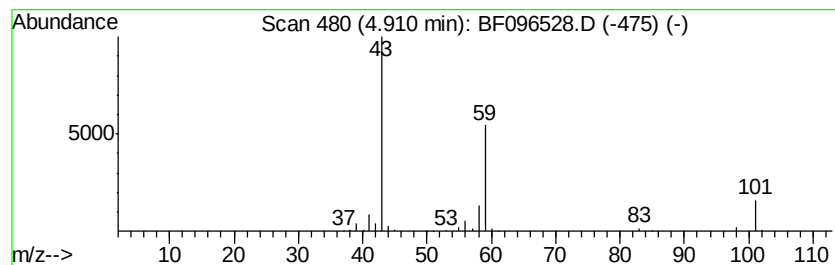
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.91 | 10.95 ng | 435674 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 3    |    | 3-Hexanol                           | 102 | C6H14O   | 000623-37-0 | 33   |
| 4    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 5    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 16   |



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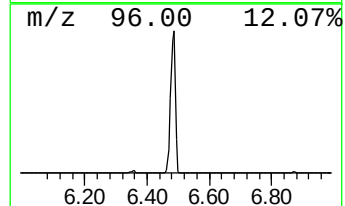
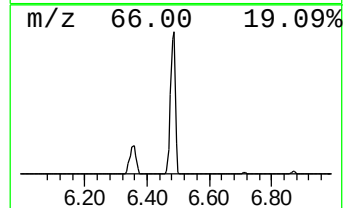
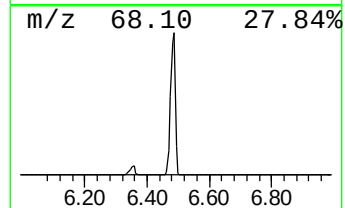
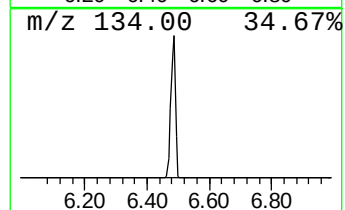
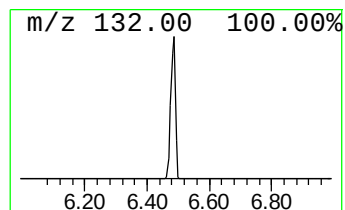
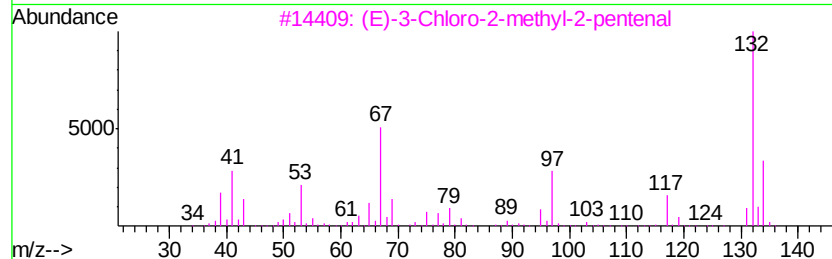
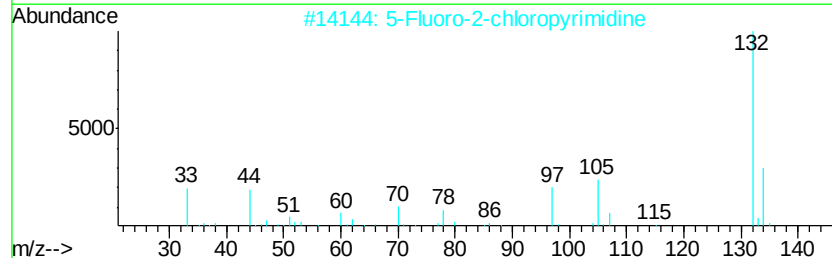
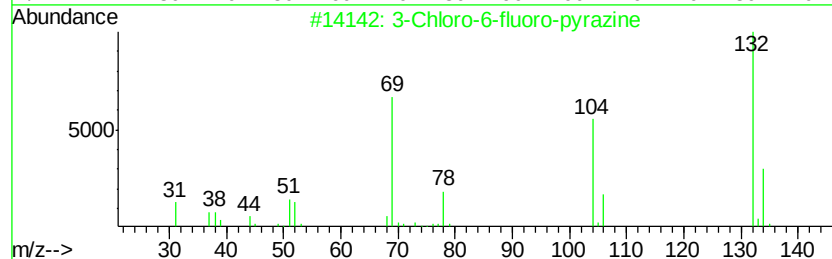
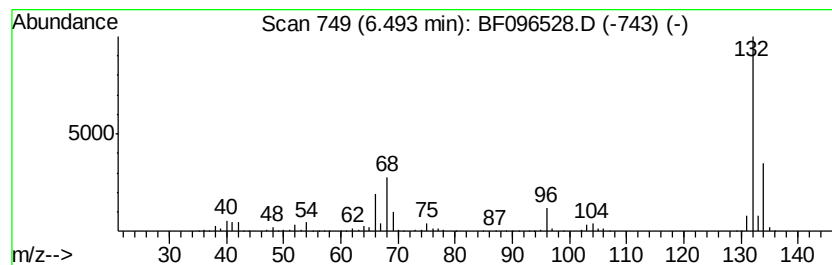
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown6.49 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.49 | 71.83 ng | 2859170 | 1,4-Dichlorobenzene-d4 | 6.71 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 17   |
| 3    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | Tranlylcypromine-propionyl       | 189 | C12H15NO  | 1000123-86-3 | 12   |



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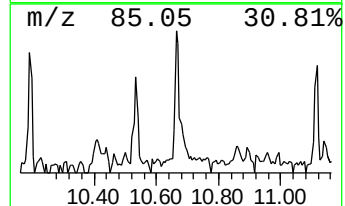
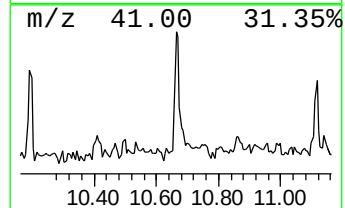
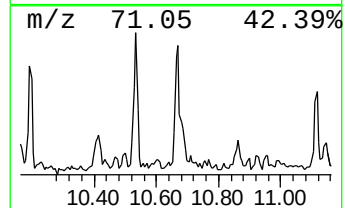
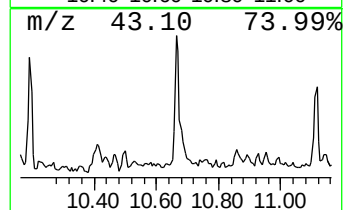
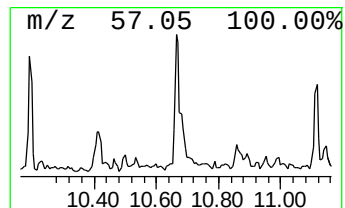
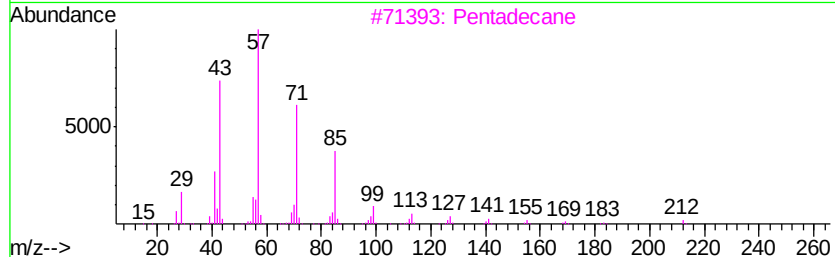
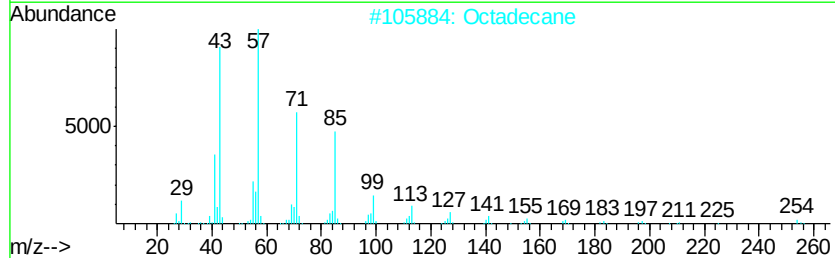
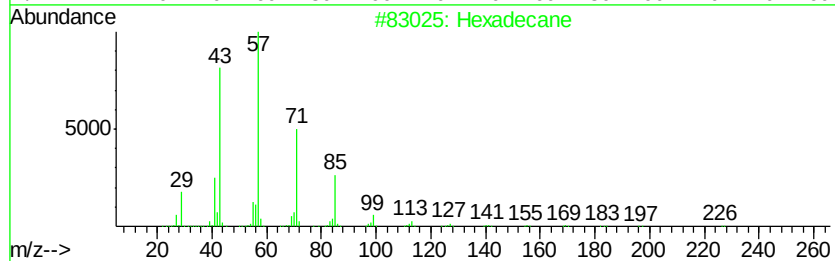
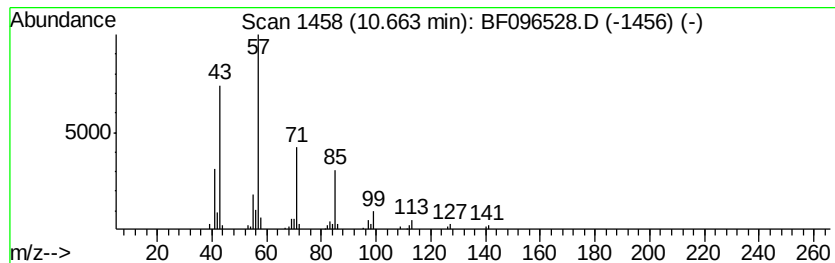
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Peak Number 5 Hexadecane Concentration Rank 6

| R.T.      | EstConc      | Area  | Relative to ISTD | R.T.        |      |
|-----------|--------------|-------|------------------|-------------|------|
| 10.66     | 2.19 ng      | 87781 | Phenanthrene-d10 | 11.23       |      |
| Hit# of 5 | Tentative ID | MW    | MolForm          | CAS#        | Qual |
| 1         | Hexadecane   | 226   | C16H34           | 000544-76-3 | 90   |
| 2         | Octadecane   | 254   | C18H38           | 000593-45-3 | 64   |
| 3         | Pentadecane  | 212   | C15H32           | 000629-62-9 | 59   |
| 4         | Eicosane     | 282   | C20H42           | 000112-95-8 | 59   |
| 5         | Tetracosane  | 338   | C24H50           | 000646-31-1 | 59   |



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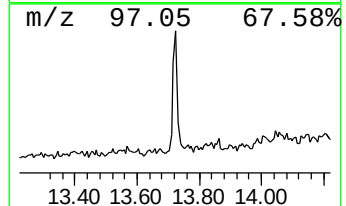
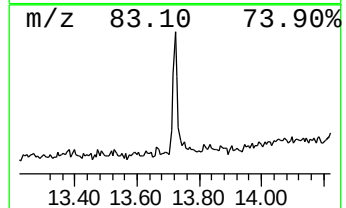
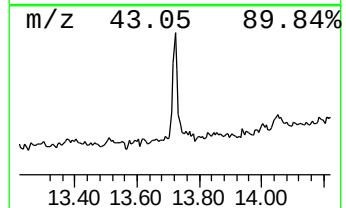
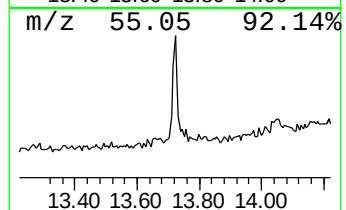
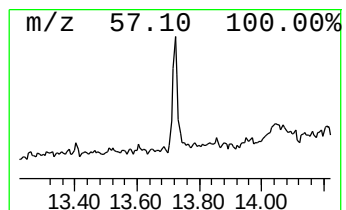
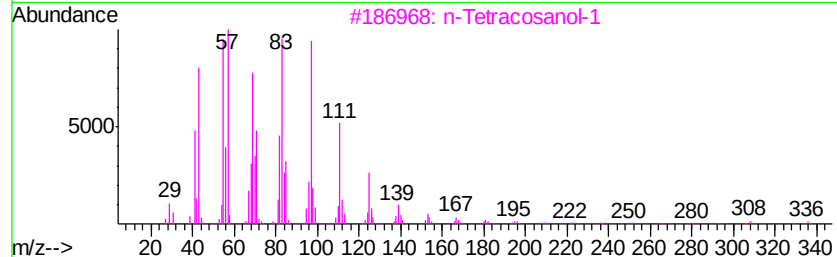
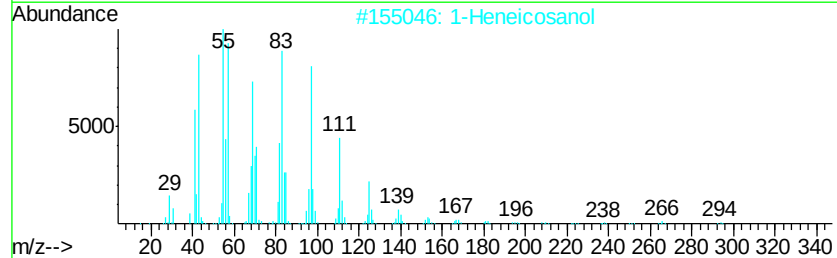
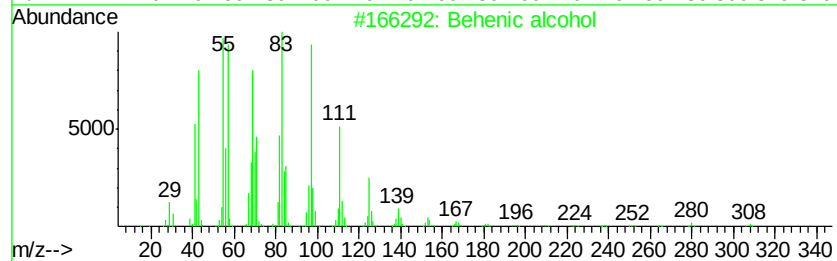
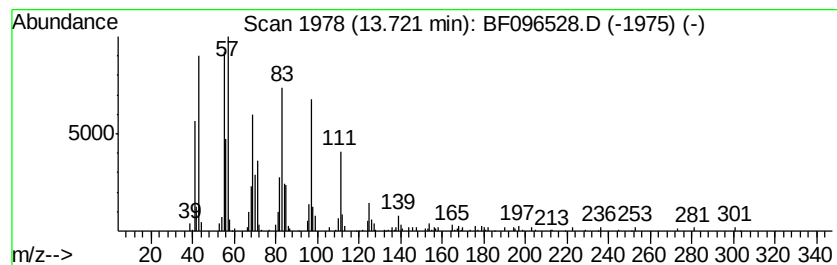
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Peak Number 6 Behenic alcohol Concentration Rank 4

| R.T.      | EstConc                     | Area   | Relative to ISTD |              | R.T.  |
|-----------|-----------------------------|--------|------------------|--------------|-------|
| 13.72     | 5.21 ng                     | 188806 | Chrysene-d12     |              | 13.86 |
| Hit# of 5 | Tentative ID                | MW     | MolForm          | CAS#         | Qual  |
| 1         | Behenic alcohol             | 326    | C22H46O          | 000661-19-8  | 93    |
| 2         | 1-Heneicosanol              | 312    | C21H44O          | 015594-90-8  | 93    |
| 3         | n-Tetracosanol-1            | 354    | C24H50O          | 000506-51-4  | 90    |
| 4         | Heptadecyl trifluoroacetate | 352    | C19H35F3O2       | 1000351-87-0 | 90    |
| 5         | n-Nonadecanol-1             | 284    | C19H40O          | 001454-84-8  | 90    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF070617\  
Data File : BF096528.D  
Acq On : 6 Jul 2017 12:59  
Operator : SJ/MA  
Sample : I4053-01  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
CL-02-070317-A

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF070117.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 |
| (S)-(+)-1,2-Propa... | 3.08  | 2.3     | ng    | 89856    | 1                     | 6.71  | 796113 | 20.0 |
| 2-Pentanone, 4-hy... | 4.91  | 10.9    | ng    | 435674   | 1                     | 6.71  | 796113 | 20.0 |
| unknown6.49          | 6.49  | 71.8    | ng    | 2859170  | 1                     | 6.71  | 796113 | 20.0 |
| Hexadecane           | 10.66 | 2.2     | ng    | 87781    | 4                     | 11.23 | 802954 | 20.0 |
| Behenic alcohol      | 13.72 | 5.2     | ng    | 188806   | 5                     | 13.86 | 724940 | 20.0 |