

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071917\  
 Data File : BF096873.D  
 Acq On : 19 Jul 2017 16:43  
 Operator : SJ/JU  
 Sample : I4272-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 HDD-P1LWC2

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-BF071317.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         | 2.851       | 146           | 147         | 160          | rBV5     | 24089          | 60000         | 2.01%           | 0.252%        |
| 2         | 4.769       | 462           | 473         | 487          | rVB      | 176876         | 310100        | 10.40%          | 1.302%        |
| 3         | 5.198       | 541           | 546         | 549          | rBV      | 2613602        | 2745287       | 92.04%          | 11.528%       |
| 4         | 6.239       | 717           | 723         | 733          | rBV      | 2285888        | 2982610       | 100.00%         | 12.525%       |
| 5         | 6.357       | 738           | 743         | 747          | rBV      | 2537513        | 2753747       | 92.33%          | 11.563%       |
| 6         | 6.587       | 778           | 782         | 785          | rBV      | 627053         | 537490        | 18.02%          | 2.257%        |
| 7         | 6.745       | 804           | 809         | 812          | rBV      | 1898136        | 1906092       | 63.91%          | 8.004%        |
| 8         | 7.151       | 872           | 878         | 881          | rBV      | 1592695        | 1669708       | 55.98%          | 7.011%        |
| 9         | 7.869       | 995           | 1000        | 1003         | rBV      | 804794         | 729317        | 24.45%          | 3.063%        |
| 10        | 8.945       | 1177          | 1183        | 1186         | rBV      | 2464011        | 2563965       | 85.96%          | 10.767%       |
| 11        | 9.339       | 1246          | 1250        | 1254         | rBV      | 373538         | 324604        | 10.88%          | 1.363%        |
| 12        | 9.616       | 1292          | 1297        | 1301         | rVB      | 862753         | 801280        | 26.87%          | 3.365%        |
| 13        | 10.069      | 1370          | 1374        | 1376         | rVB      | 38596          | 33411         | 1.12%           | 0.140%        |
| 14        | 10.404      | 1425          | 1431        | 1434         | rBV      | 1747337        | 1764811       | 59.17%          | 7.411%        |
| 15        | 10.539      | 1451          | 1454        | 1461         | rVB      | 47914          | 55496         | 1.86%           | 0.233%        |
| 16        | 10.986      | 1522          | 1530        | 1532         | rBV2     | 25348          | 30376         | 1.02%           | 0.128%        |
| 17        | 11.092      | 1542          | 1548        | 1551         | rBV      | 960348         | 802538        | 26.91%          | 3.370%        |
| 18        | 11.639      | 1638          | 1641        | 1651         | rBV2     | 63384          | 82104         | 2.75%           | 0.345%        |
| 19        | 12.680      | 1811          | 1818        | 1821         | rBV      | 2305503        | 2312750       | 77.54%          | 9.712%        |
| 20        | 13.586      | 1963          | 1972        | 1978         | rBV2     | 116483         | 153402        | 5.14%           | 0.644%        |
| 21        | 13.715      | 1989          | 1994        | 1998         | rBV      | 774162         | 694709        | 23.29%          | 2.917%        |
| 22        | 15.086      | 2222          | 2227        | 2232         | rBV      | 430846         | 470197        | 15.76%          | 1.974%        |
| 23        | 15.568      | 2304          | 2309        | 2315         | rVB7     | 18135          | 30161         | 1.01%           | 0.127%        |

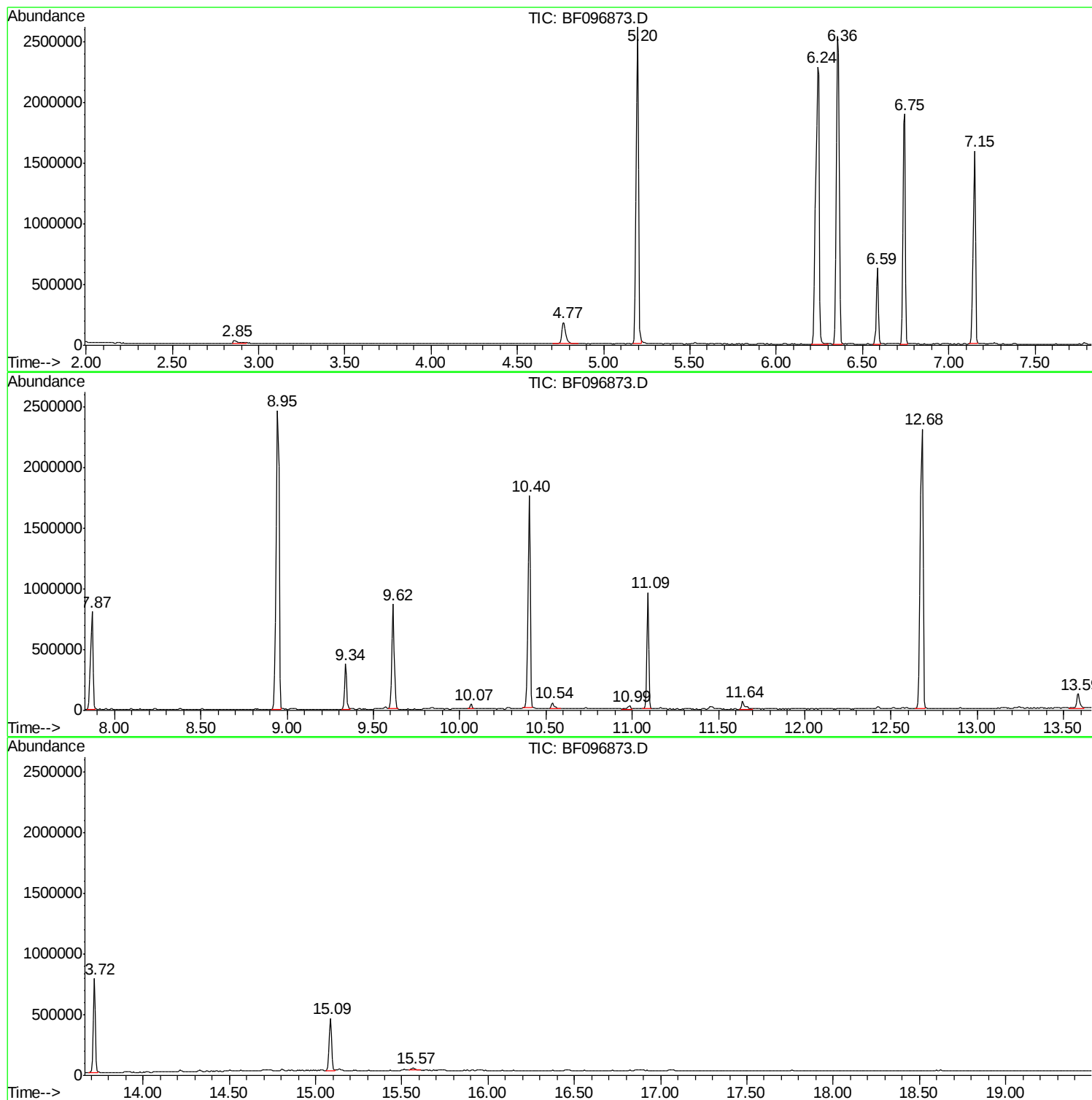
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BNA\_F  
ClientSampleId :  
HDD-P1LWC2

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF071317.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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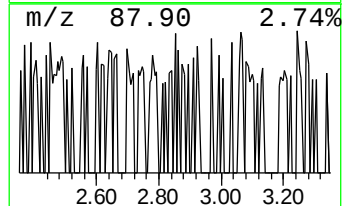
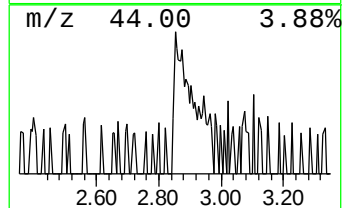
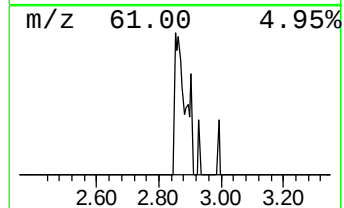
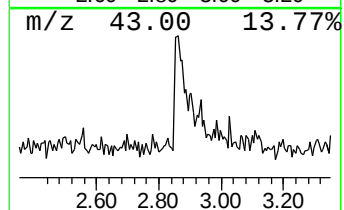
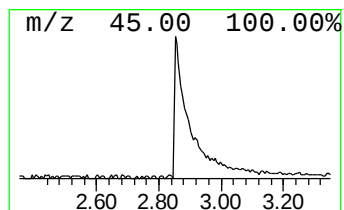
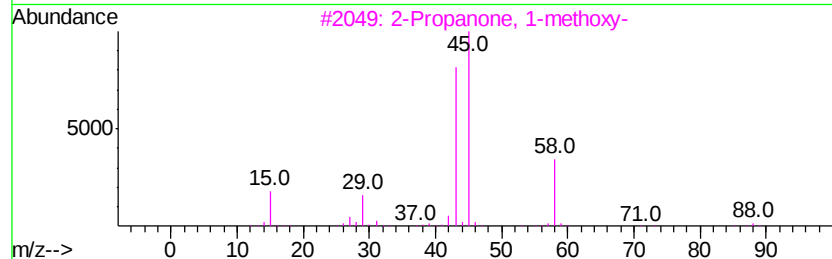
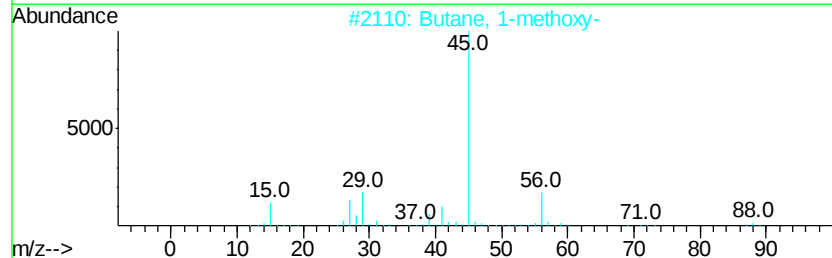
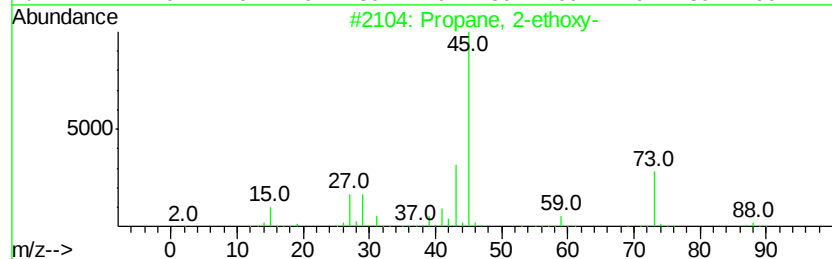
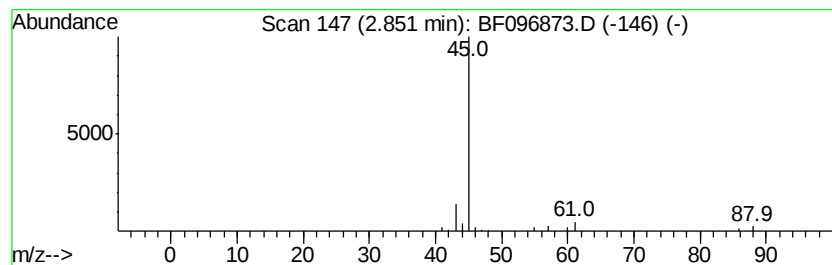
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.85 Concentration Rank 5

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 2.85 | 2.23 ng | 60000 | 1,4-Dichlorobenzene-d4 | 6.59 |

| Hit# | of | Tentative ID            | MW | MolForm | CAS#        | Qual |
|------|----|-------------------------|----|---------|-------------|------|
| 1    | 5  | Propane, 2-ethoxy-      | 88 | C5H12O  | 000625-54-7 | 9    |
| 2    |    | Butane, 1-methoxy-      | 88 | C5H12O  | 000628-28-4 | 9    |
| 3    |    | 2-Propanone, 1-methoxy- | 88 | C4H8O2  | 005878-19-3 | 9    |
| 4    |    | R-(-)-1,2-propanediol   | 76 | C3H8O2  | 004254-14-2 | 9    |
| 5    |    | 2-Butanol, (R)-         | 74 | C4H10O  | 014898-79-4 | 9    |



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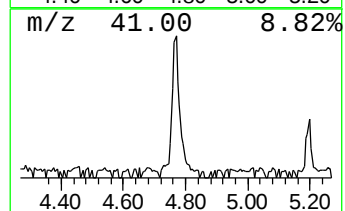
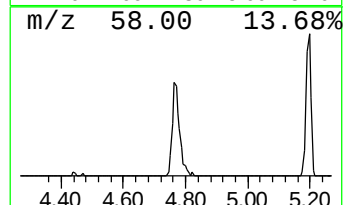
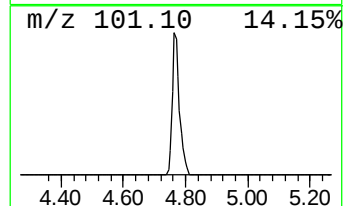
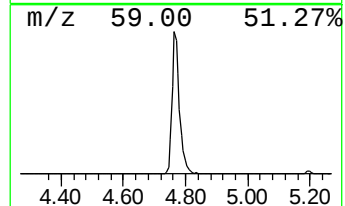
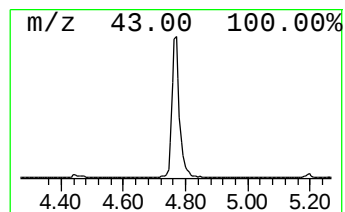
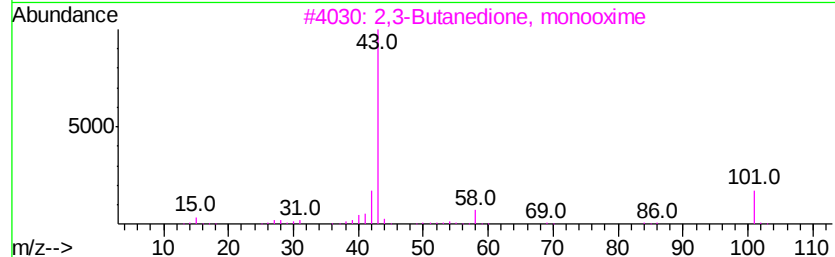
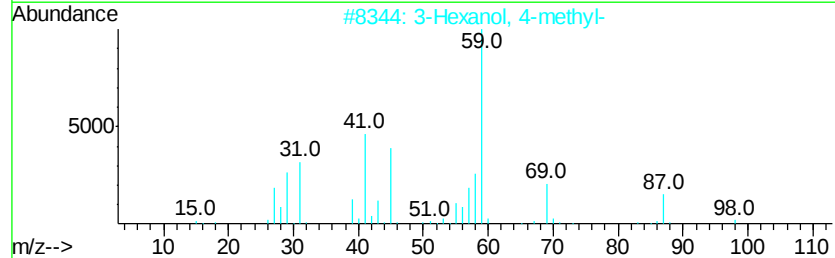
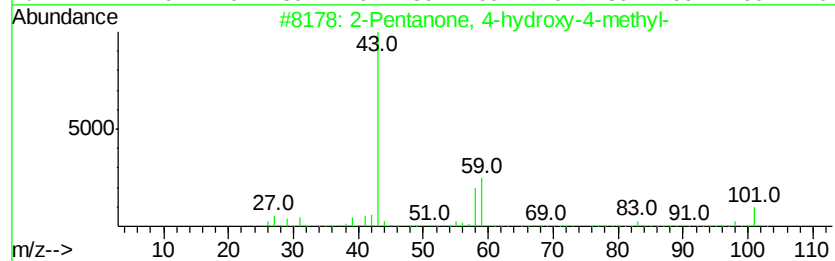
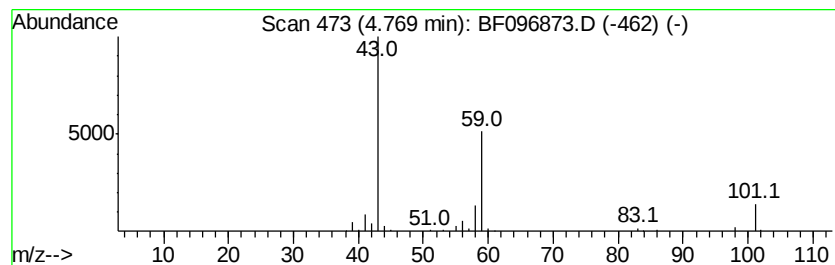
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TIC Integration Parameters: LSCINT.P

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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. |
|------|----------|--------|------------------------|------|
| 4.77 | 11.54 ng | 310100 | 1,4-Dichlorobenzene-d4 | 6.59 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 59   |
| 2    |    | 3-Hexanol, 4-methyl-                | 116 | C7H16O  | 000615-29-2 | 40   |
| 3    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 38   |
| 4    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 28   |
| 5    |    | 2-Hexanol, 2-methyl-                | 116 | C7H16O  | 000625-23-0 | 28   |



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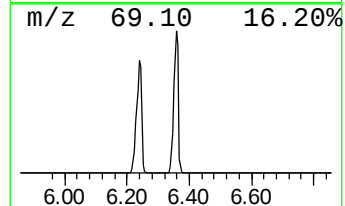
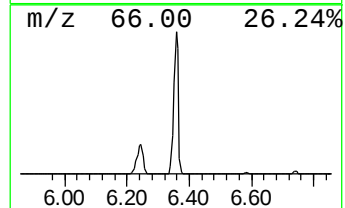
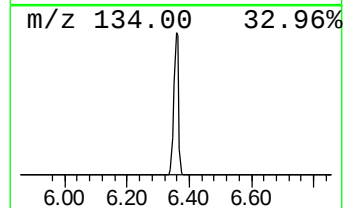
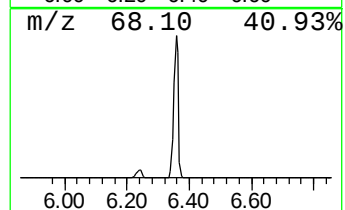
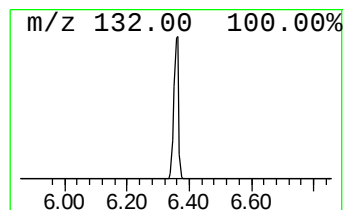
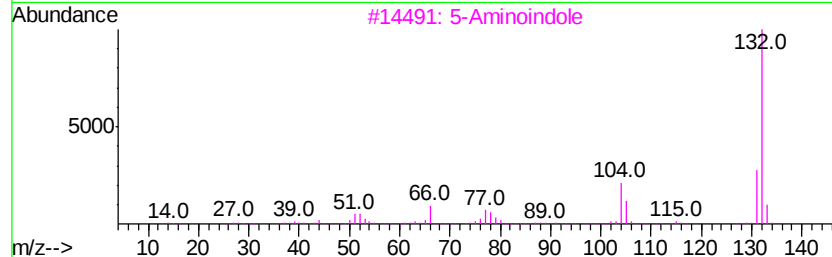
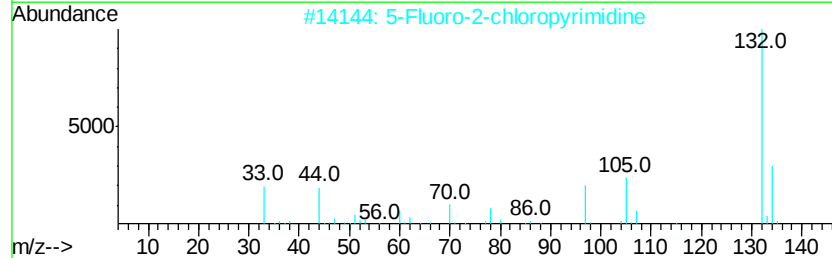
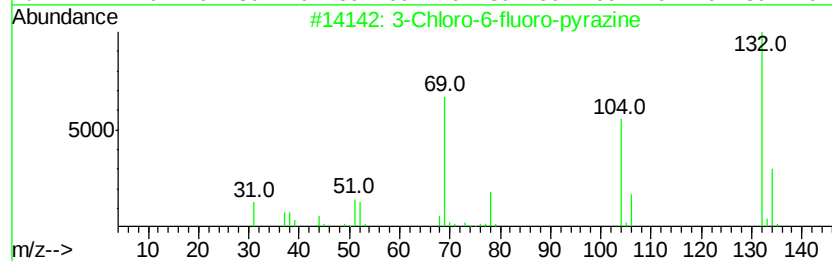
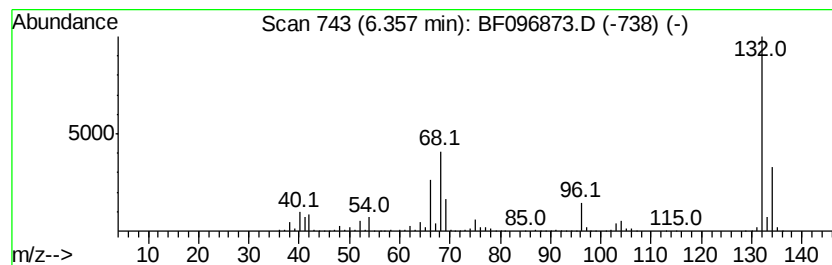
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown6.36 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 6.36 | 102.47 ng | 2753750 | 1,4-Dichlorobenzene-d4 | 6.59 |

| 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    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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Instrument :  
BNA\_F  
ClientSampleId :  
HDD-P1LWC2

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF071317.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

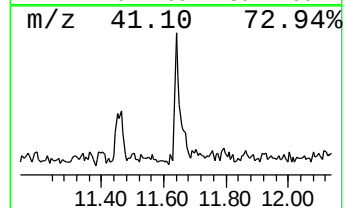
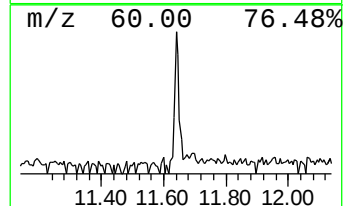
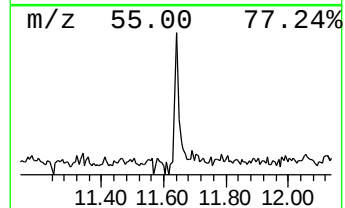
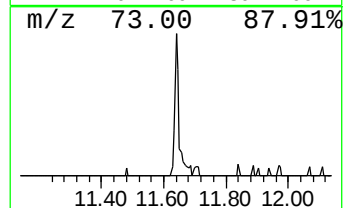
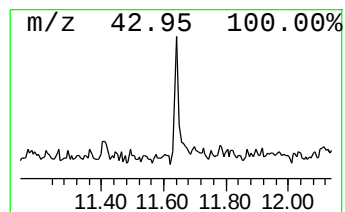
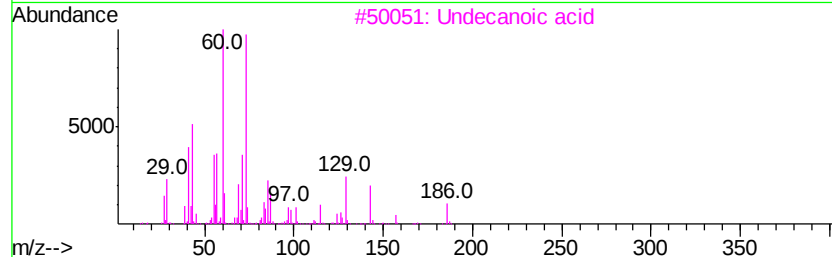
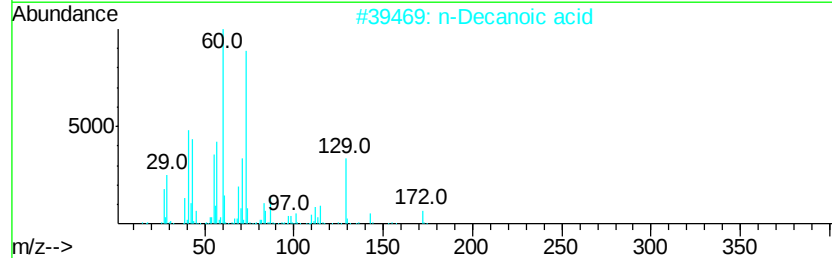
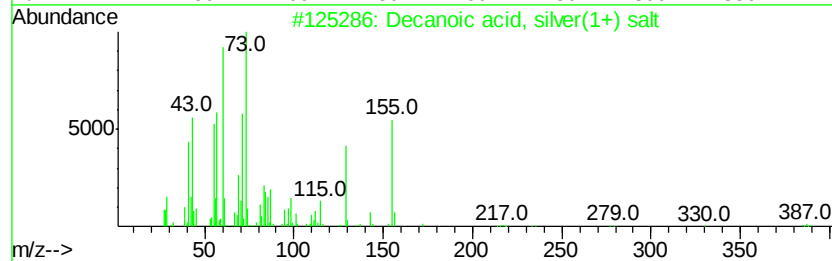
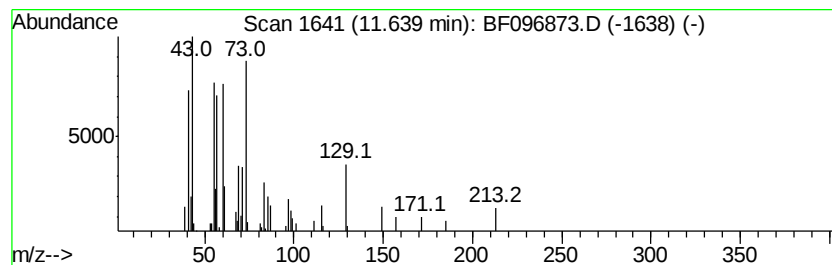
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Decanoic acid, silver(1+) salt Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 11.64 | 2.05 ng | 82104 | Phenanthrene-d10 | 11.09 |

| Hit# | of | Tentative ID                   | MW  | MolForm    | CAS#        | Qual |
|------|----|--------------------------------|-----|------------|-------------|------|
| 1    | 5  | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 53   |
| 2    |    | n-Decanoic acid                | 172 | C10H20O2   | 000334-48-5 | 50   |
| 3    |    | Undecanoic acid                | 186 | C11H22O2   | 000112-37-8 | 45   |
| 4    |    | 11-Bromoundecanoic acid        | 264 | C11H21BrO2 | 002834-05-1 | 43   |
| 5    |    | Nonanoic acid                  | 158 | C9H18O2    | 000112-05-0 | 43   |



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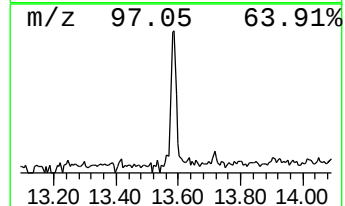
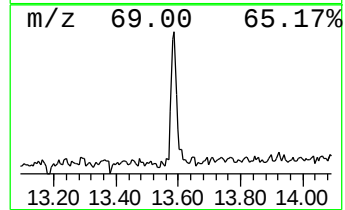
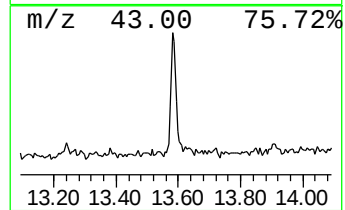
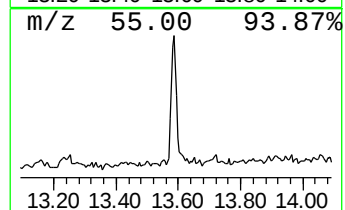
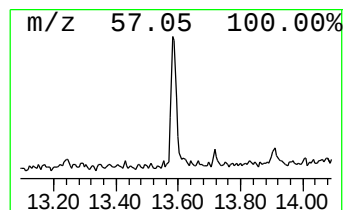
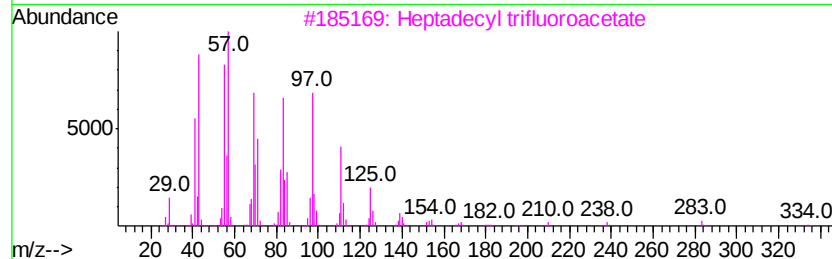
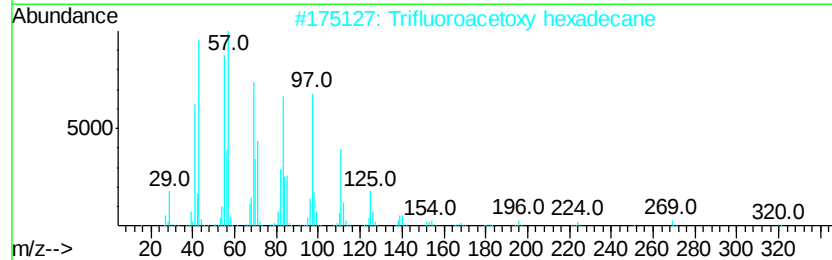
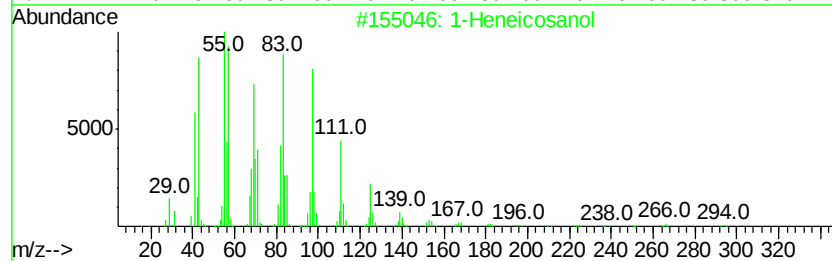
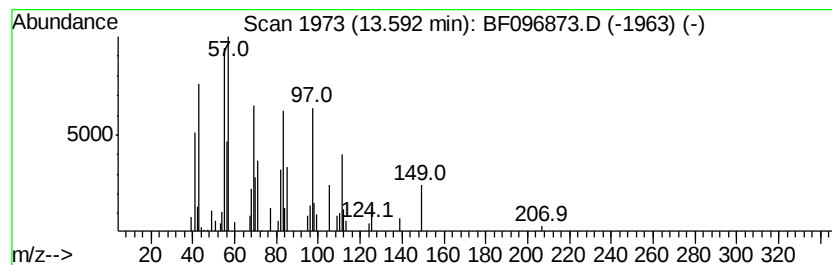
Instrument :  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 1-Heneicosanol Concentration Rank 4

| R.T.      | EstConc                     | Area   | Relative to ISTD | R.T.         |      |
|-----------|-----------------------------|--------|------------------|--------------|------|
| 13.59     | 4.42 ng                     | 153402 | Chrysene-d12     | 13.72        |      |
| Hit# of 5 | Tentative ID                | MW     | MolForm          | CAS#         | Qual |
| 1         | 1-Heneicosanol              | 312    | C21H44O          | 015594-90-8  | 95   |
| 2         | Trifluoroacetoxy hexadecane | 338    | C18H33F3O2       | 006222-03-3  | 94   |
| 3         | Heptadecyl trifluoroacetate | 352    | C19H35F3O2       | 1000351-87-0 | 94   |
| 4         | n-Tetracosanol-1            | 354    | C24H50O          | 000506-51-4  | 93   |
| 5         | Behenic alcohol             | 326    | C22H46O          | 000661-19-8  | 93   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF071917\  
Data File : BF096873.D  
Acq On : 19 Jul 2017 16:43  
Operator : SJ/JU  
Sample : I4272-01  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
HDD-P1LWC2

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF071317.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 |
| unknown2.85          | 2.85  | 2.2     | ng    | 60000    | 1                     | 6.59  | 537490 | 20.0 |
| 2-Pentanone, 4-hy... | 4.77  | 11.5    | ng    | 310100   | 1                     | 6.59  | 537490 | 20.0 |
| unknown6.36          | 6.36  | 102.5   | ng    | 2753750  | 1                     | 6.59  | 537490 | 20.0 |
| Decanoic acid, si... | 11.64 | 2.0     | ng    | 82104    | 4                     | 11.09 | 802538 | 20.0 |
| 1-Heneicosanol       | 13.59 | 4.4     | ng    | 153402   | 5                     | 13.72 | 694709 | 20.0 |