

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF092723\  
 Data File : BF135481.D  
 Acq On : 27 Sep 2023 19:36  
 Operator : CG\JU  
 Sample : 04601-01  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-1

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:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135481.D\data.ms

| 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         | 4.998       | 492           | 495         | 504          | rBV      | 29214          | 44518         | 1.14%           | 0.168%        |
| 2         | 5.387       | 557           | 561         | 587          | rBV      | 3449044        | 3847976       | 98.41%          | 14.496%       |
| 3         | 6.398       | 729           | 733         | 761          | rBV      | 3440471        | 3910170       | 100.00%         | 14.730%       |
| 4         | 6.598       | 761           | 767         | 784          | rBV2     | 18857          | 66536         | 1.70%           | 0.251%        |
| 5         | 6.751       | 790           | 793         | 801          | rBV      | 1078666        | 928941        | 23.76%          | 3.499%        |
| 6         | 7.316       | 885           | 889         | 902          | rBV      | 2306338        | 2517288       | 64.38%          | 9.483%        |
| 7         | 8.034       | 1007          | 1011        | 1030         | rVB      | 1278446        | 1202395       | 30.75%          | 4.530%        |
| 8         | 9.110       | 1189          | 1194        | 1197         | rBV      | 3940021        | 3744841       | 95.77%          | 14.107%       |
| 9         | 9.228       | 1211          | 1214        | 1223         | rVB      | 54675          | 72345         | 1.85%           | 0.273%        |
| 10        | 9.786       | 1305          | 1309        | 1322         | rVB      | 1356148        | 1223426       | 31.29%          | 4.609%        |
| 11        | 10.586      | 1441          | 1445        | 1462         | rBV      | 2060398        | 2129556       | 54.46%          | 8.022%        |
| 12        | 11.280      | 1560          | 1563        | 1566         | rBV      | 1249647        | 1120787       | 28.66%          | 4.222%        |
| 13        | 11.304      | 1566          | 1567        | 1571         | rVB      | 68089          | 51541         | 1.32%           | 0.194%        |
| 14        | 11.822      | 1652          | 1655        | 1666         | rBV2     | 170375         | 241702        | 6.18%           | 0.911%        |
| 15        | 12.504      | 1768          | 1771        | 1775         | rBV      | 129528         | 112367        | 2.87%           | 0.423%        |
| 16        | 12.610      | 1786          | 1789        | 1794         | rBV3     | 38470          | 50561         | 1.29%           | 0.190%        |
| 17        | 12.733      | 1803          | 1810        | 1816         | rBV      | 111118         | 118339        | 3.03%           | 0.446%        |
| 18        | 12.880      | 1830          | 1835        | 1838         | rBV      | 3021099        | 2755573       | 70.47%          | 10.381%       |
| 19        | 13.939      | 2000          | 2015        | 2019         | rBV      | 809481         | 930851        | 23.81%          | 3.507%        |
| 20        | 14.416      | 2090          | 2096        | 2101         | rBV3     | 28634          | 43268         | 1.11%           | 0.163%        |
| 21        | 14.704      | 2140          | 2145        | 2152         | rBV      | 228558         | 318622        | 8.15%           | 1.200%        |
| 22        | 14.986      | 2189          | 2193        | 2201         | rBV2     | 52929          | 100980        | 2.58%           | 0.380%        |
| 23        | 15.286      | 2240          | 2244        | 2248         | rBV      | 34542          | 40227         | 1.03%           | 0.152%        |
| 24        | 15.351      | 2251          | 2255        | 2259         | rVB      | 48138          | 57853         | 1.48%           | 0.218%        |
| 25        | 15.410      | 2260          | 2265        | 2277         | rBV      | 666469         | 871497        | 22.29%          | 3.283%        |
| 26        | 15.868      | 2340          | 2343        | 2350         | rVB3     | 30038          | 43441         | 1.11%           | 0.164%        |

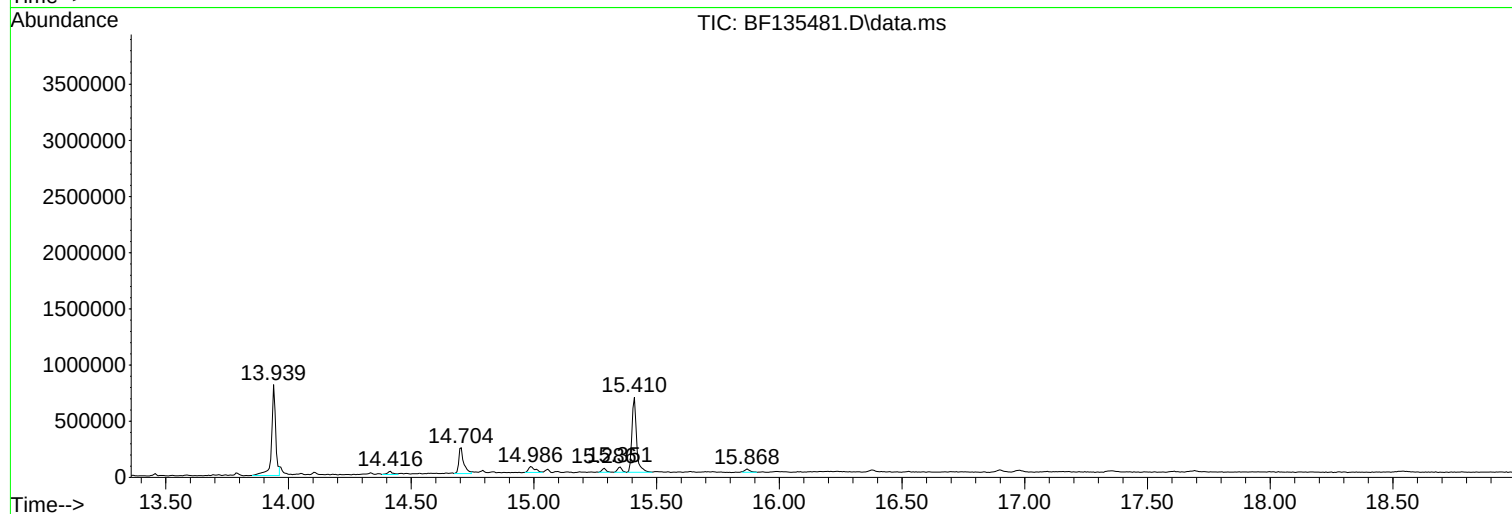
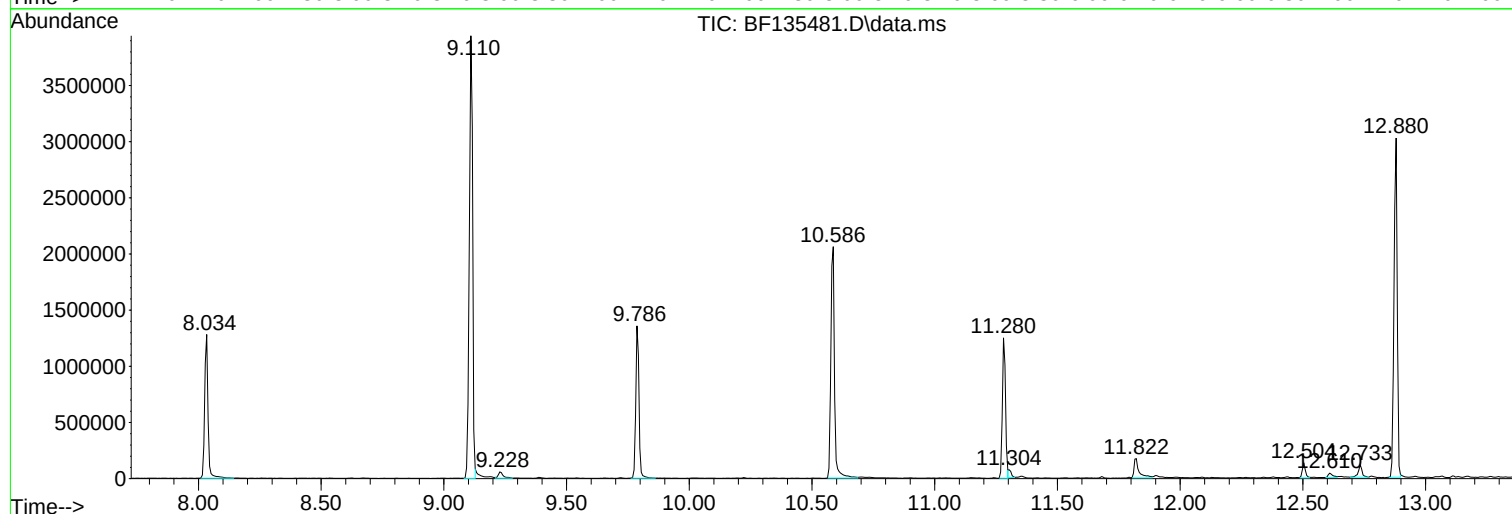
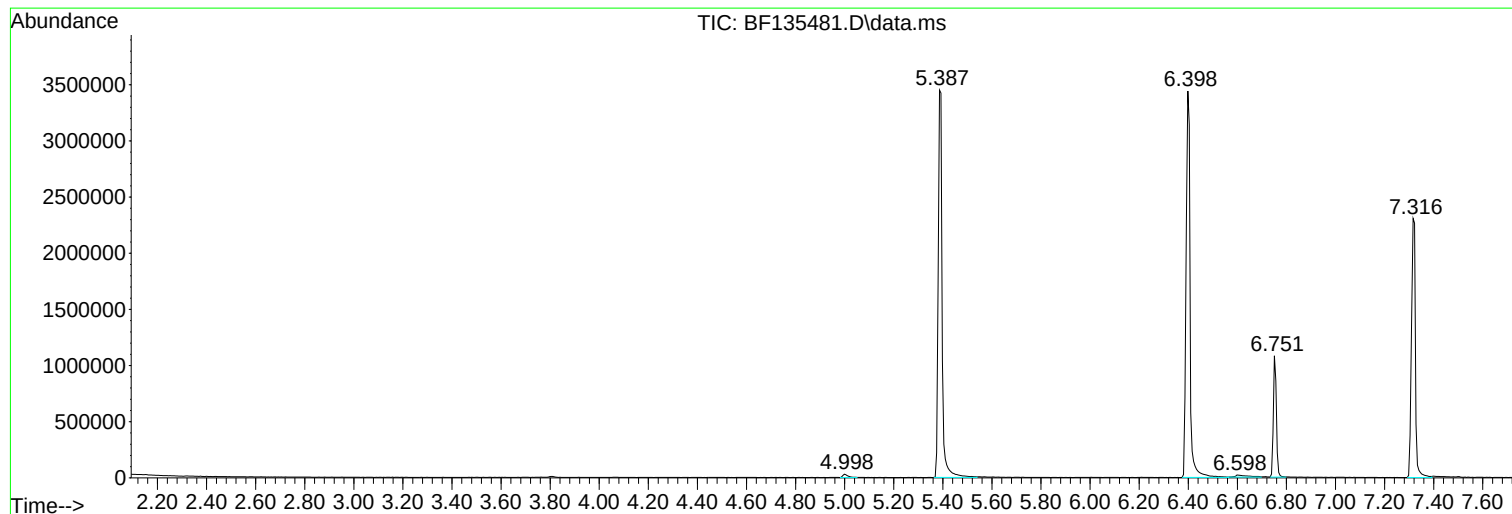
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Instrument :  
BNA\_F  
ClientSampleId :  
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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BNA\_F  
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TP-1

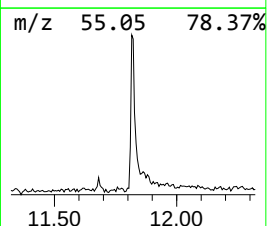
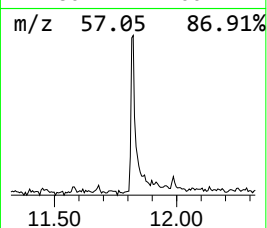
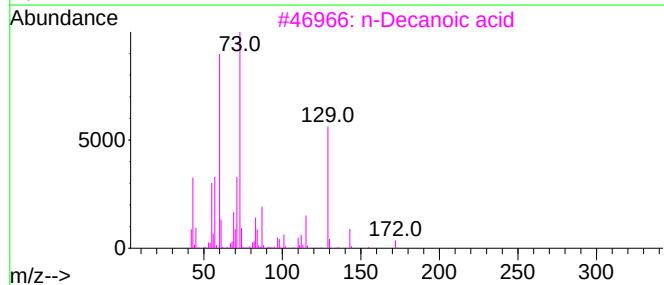
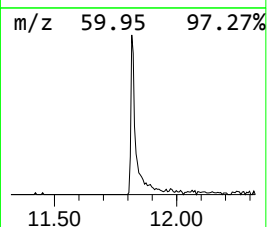
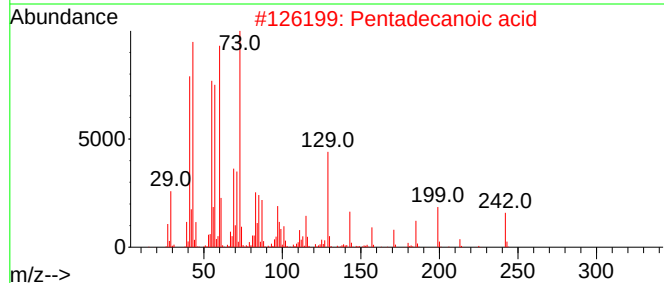
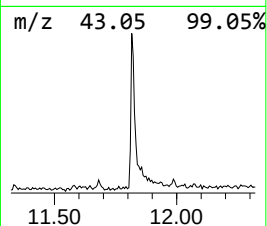
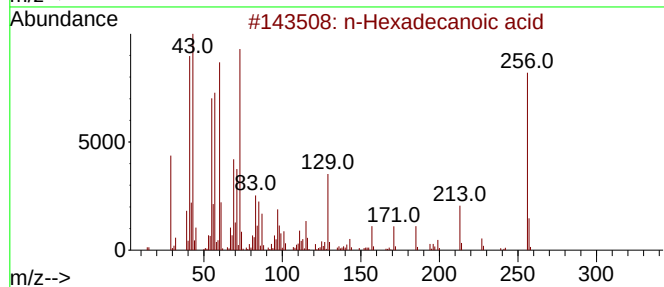
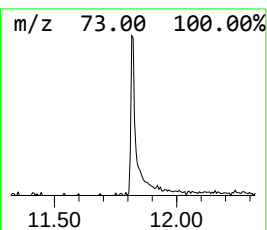
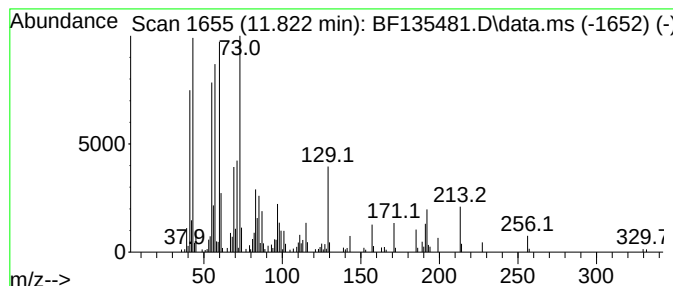
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.822 | 4.31 ng | 241702 | Phenanthrene-d10 | 11.281 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 3    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 83   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 5    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |



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BNA\_F  
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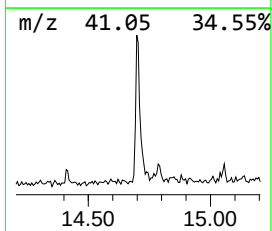
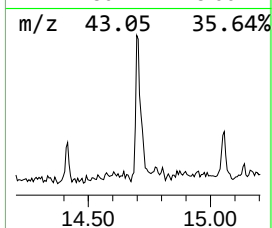
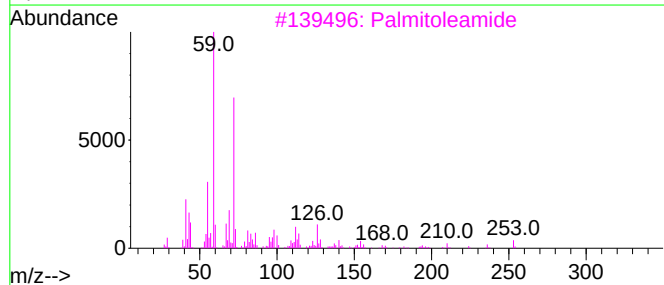
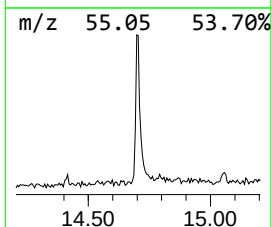
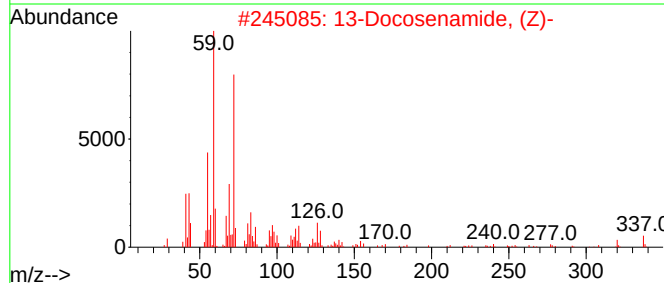
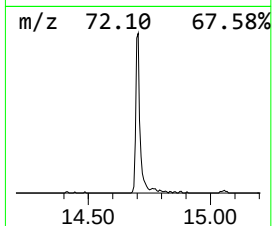
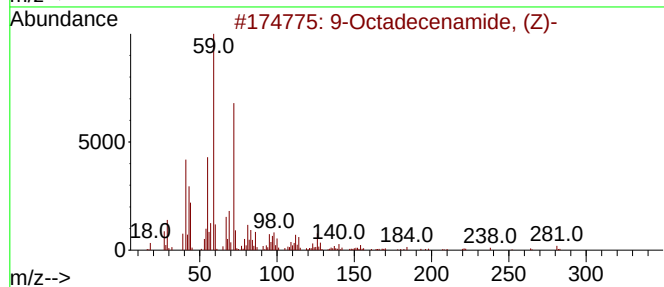
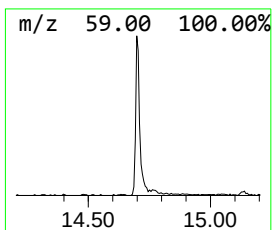
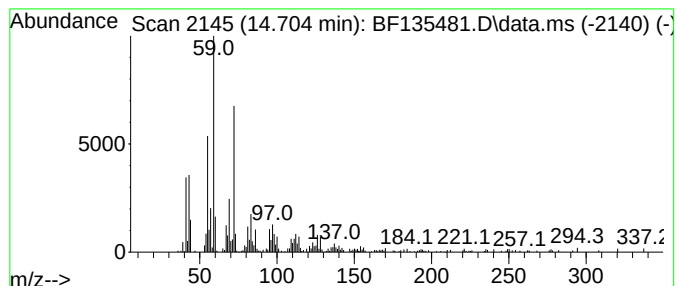
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 9-Octadecenamide, (Z)- Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.704 | 7.31 ng | 318622 | Perylene-d12     | 15.410 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|------|-------------------------------------|-----|------------|-------------|------|
| 1    |      | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 91   |
| 2    |      | 13-Docosenamide, (Z)-               | 337 | C22H43NO   | 000112-84-5 | 90   |
| 3    |      | Palmitoleamide                      | 253 | C16H31NO   | 106010-22-4 | 72   |
| 4    |      | Hexadecanamide                      | 255 | C16H33NO   | 000629-54-9 | 72   |
| 5    |      | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FN03 | 061338-98-5 | 59   |



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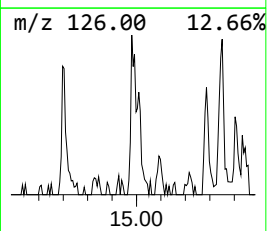
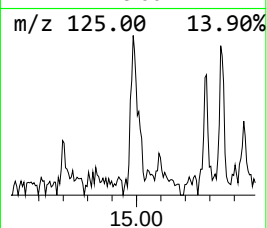
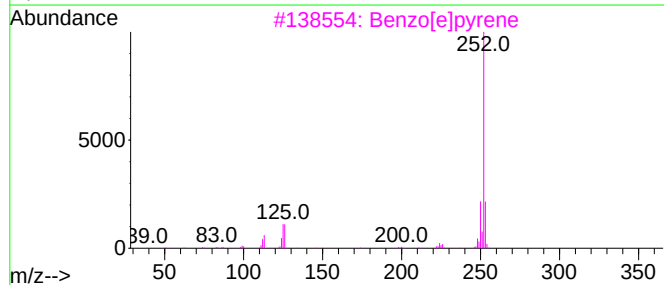
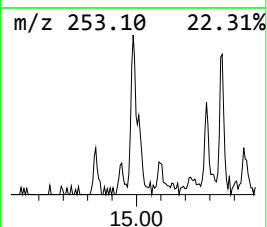
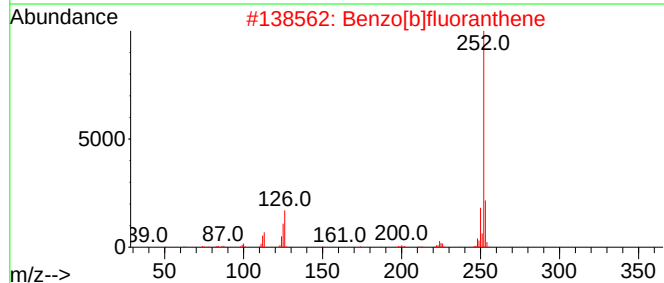
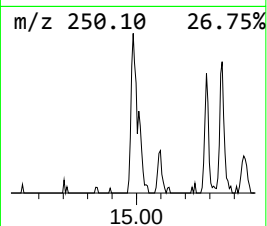
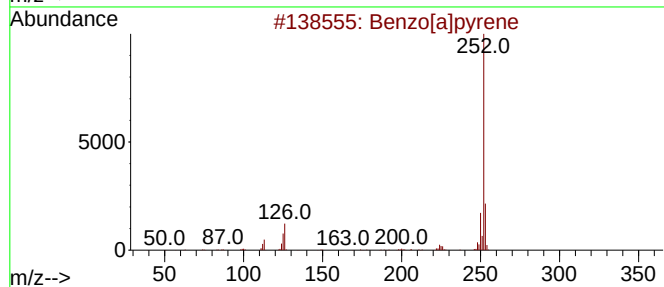
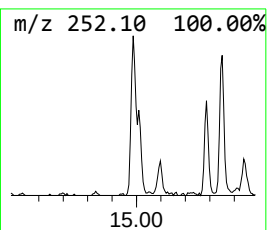
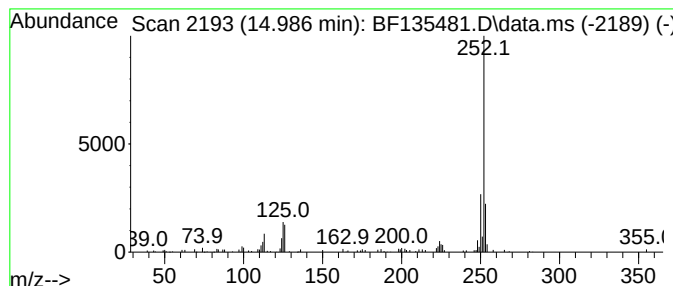
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Benzo[e]pyrene Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.986 | 2.32 ng | 100980 | Perylene-d12     | 15.410 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Benzo[a]pyrene       | 252 | C20H12  | 000050-32-8 | 95   |
| 2    |    |   | Benzo[b]fluoranthene | 252 | C20H12  | 000205-99-2 | 94   |
| 3    |    |   | Benzo[e]pyrene       | 252 | C20H12  | 000192-97-2 | 93   |
| 4    |    |   | Benzo[k]fluoranthene | 252 | C20H12  | 000207-08-9 | 89   |
| 5    |    |   | Benzo[j]fluoranthene | 252 | C20H12  | 000205-82-3 | 89   |



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Misc :  
ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF091123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| n-Hexadecanoic ... | 11.822 | 4.3     | ng    | 241702   | 4                     | 11.281 | 1120790 | 20.0 |
| 9-Octadecenamid... | 14.704 | 7.3     | ng    | 318622   | 6                     | 15.410 | 871497  | 20.0 |
| Benzo[e]pyrene     | 14.986 | 2.3     | ng    | 100980   | 6                     | 15.410 | 871497  | 20.0 |