

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF081919\  
 Data File : BF116405.D  
 Acq On : 19 Aug 2019 23:17  
 Operator : HP/JU  
 Sample : K4290-02  
 Misc :  
 ALS Vial : 14 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 B-2

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-BF073019.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         | 5.428       | 565           | 568         | 600          | rBV      | 1640336        | 2250245       | 72.90%          | 8.676%        |
| 2         | 6.451       | 738           | 742         | 760          | rBV      | 2204825        | 2398592       | 77.71%          | 9.248%        |
| 3         | 6.581       | 760           | 764         | 781          | rVB      | 2367096        | 2439540       | 79.04%          | 9.406%        |
| 4         | 6.804       | 799           | 802         | 812          | rBV      | 603870         | 571552        | 18.52%          | 2.204%        |
| 5         | 6.957       | 825           | 828         | 848          | rBV      | 2079521        | 1946605       | 63.07%          | 7.505%        |
| 6         | 7.369       | 894           | 898         | 920          | rBV      | 1596424        | 1563210       | 50.64%          | 6.027%        |
| 7         | 8.081       | 1016          | 1019        | 1040         | rBV      | 709605         | 737817        | 23.90%          | 2.845%        |
| 8         | 9.151       | 1198          | 1201        | 1212         | rBV      | 3075341        | 2899730       | 93.94%          | 11.180%       |
| 9         | 9.551       | 1265          | 1269        | 1282         | rBV      | 561152         | 504775        | 16.35%          | 1.946%        |
| 10        | 9.833       | 1314          | 1317        | 1321         | rBV      | 1092879        | 889989        | 28.83%          | 3.431%        |
| 11        | 10.622      | 1448          | 1451        | 1463         | rBV      | 1740589        | 1893297       | 61.34%          | 7.300%        |
| 12        | 10.745      | 1467          | 1472        | 1479         | rVV2     | 28163          | 67946         | 2.20%           | 0.262%        |
| 13        | 10.986      | 1511          | 1513        | 1518         | rBV3     | 24674          | 33276         | 1.08%           | 0.128%        |
| 14        | 11.322      | 1566          | 1570        | 1573         | rBV      | 1063025        | 980964        | 31.78%          | 3.782%        |
| 15        | 11.774      | 1643          | 1647        | 1651         | rBV6     | 34796          | 81369         | 2.64%           | 0.314%        |
| 16        | 11.845      | 1655          | 1659        | 1667         | rBV2     | 525924         | 639869        | 20.73%          | 2.467%        |
| 17        | 12.539      | 1774          | 1777        | 1786         | rBV      | 178926         | 281574        | 9.12%           | 1.086%        |
| 18        | 12.627      | 1789          | 1792        | 1798         | rVB      | 124266         | 175767        | 5.69%           | 0.678%        |
| 19        | 12.769      | 1814          | 1816        | 1821         | rVB      | 135077         | 138632        | 4.49%           | 0.535%        |
| 20        | 12.898      | 1834          | 1838        | 1842         | rBV      | 3041426        | 3086653       | 100.00%         | 11.901%       |
| 21        | 13.786      | 1986          | 1989        | 1996         | rVB      | 272060         | 340040        | 11.02%          | 1.311%        |
| 22        | 13.921      | 2010          | 2012        | 2015         | rVB      | 117925         | 80810         | 2.62%           | 0.312%        |
| 23        | 13.963      | 2016          | 2019        | 2023         | rBV      | 827137         | 809455        | 26.22%          | 3.121%        |
| 24        | 14.774      | 2155          | 2157        | 2163         | rVB      | 200306         | 220925        | 7.16%           | 0.852%        |
| 25        | 15.421      | 2263          | 2267        | 2279         | rVB      | 536790         | 777433        | 25.19%          | 2.998%        |
| 26        | 16.474      | 2443          | 2446        | 2454         | rVB2     | 76987          | 125845        | 4.08%           | 0.485%        |

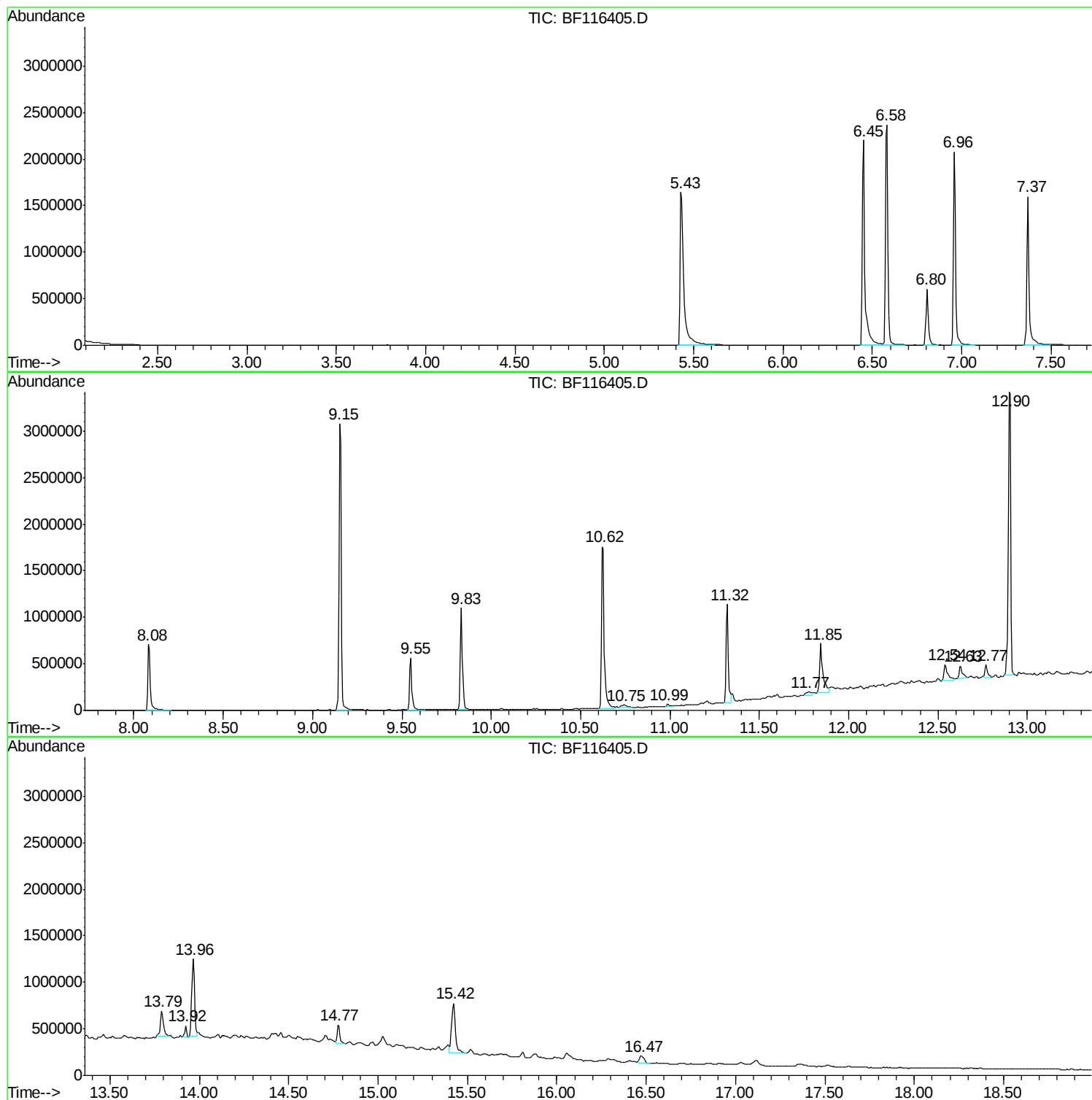
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Instrument :  
BNA\_F  
ClientSampled :  
B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.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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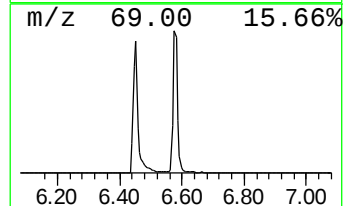
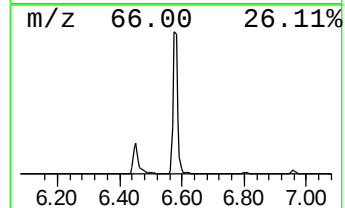
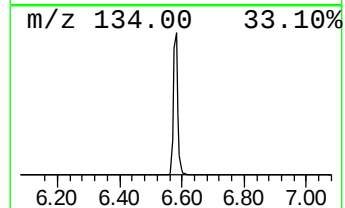
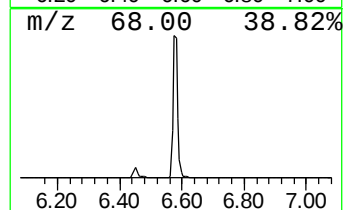
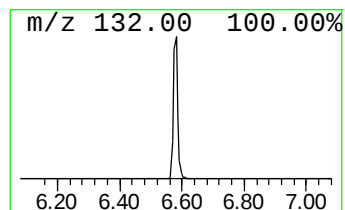
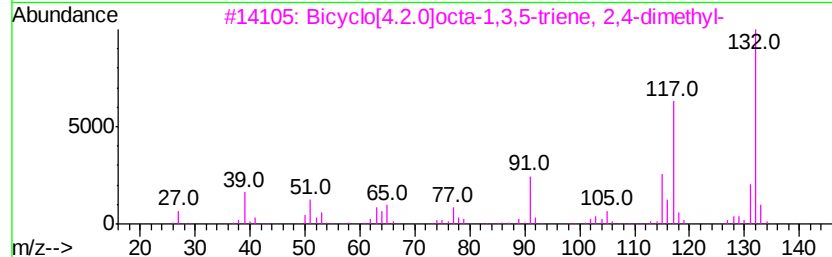
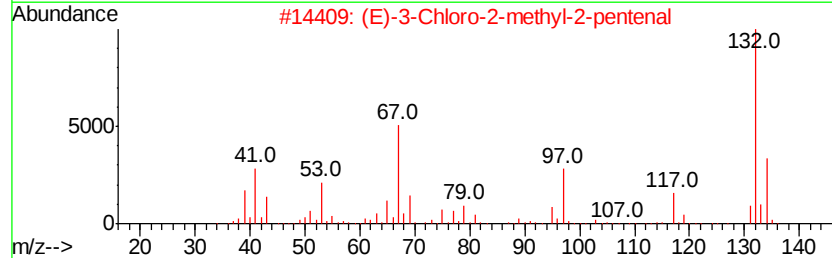
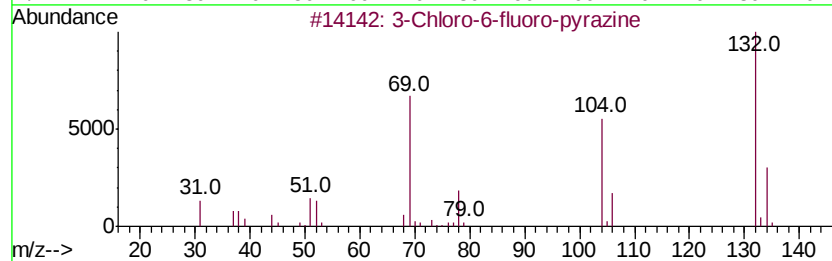
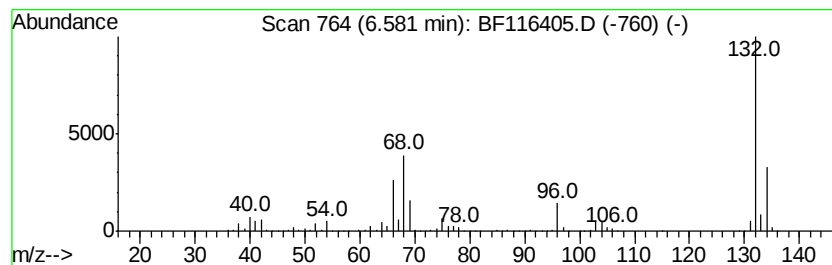
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown6.58 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.58 | 85.37 ng | 2439540 | 1,4-Dichlorobenzene-d4 | 6.80 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 12   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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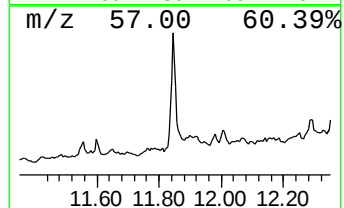
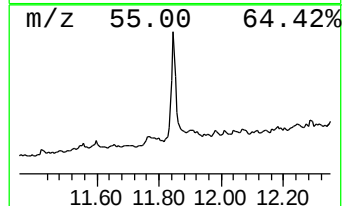
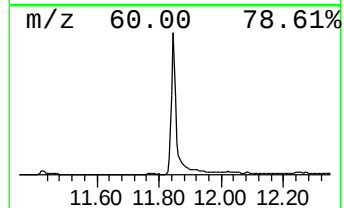
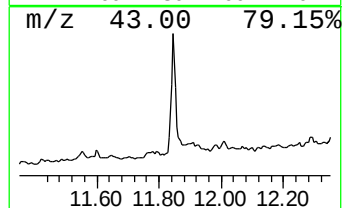
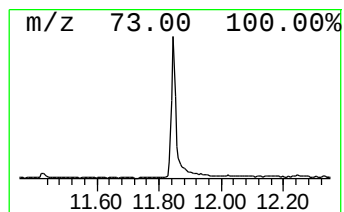
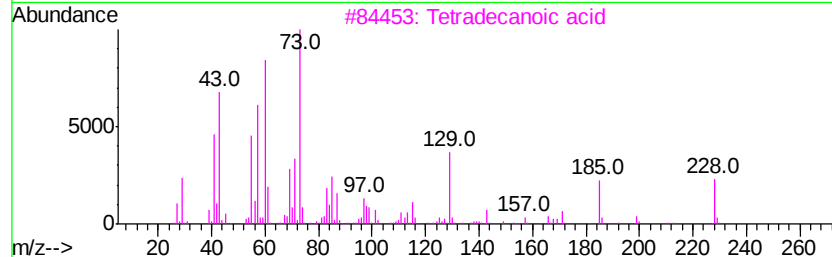
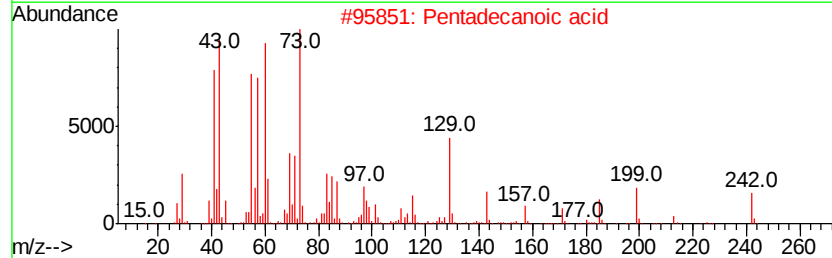
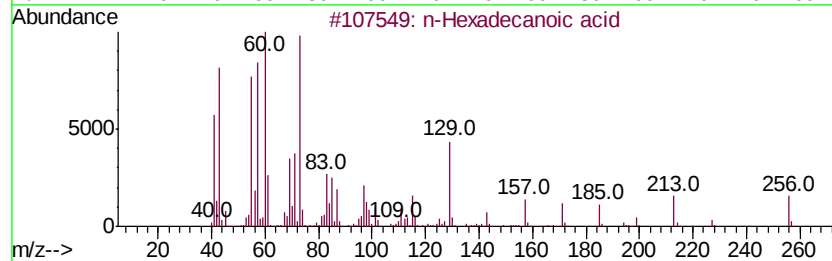
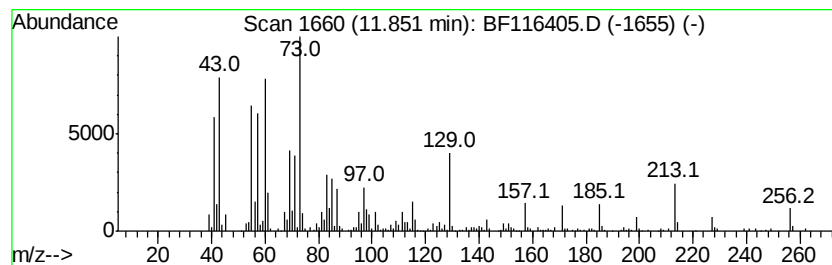
Instrument :  
BNA\_F  
ClientSampleId :  
B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.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 3 n-Hexadecanoic acid Concentration Rank 3

| R.T.    | EstConc  | Area                | Relative to ISTD |          | R.T.        |      |
|---------|----------|---------------------|------------------|----------|-------------|------|
| 11.85   | 13.05 ng | 639869              | Phenanthrene-d10 |          | 11.32       |      |
| Hit# of | 5        | Tentative ID        | MW               | MolForm  | CAS#        | Qual |
| 1       |          | n-Hexadecanoic acid | 256              | C16H32O2 | 000057-10-3 | 99   |
| 2       |          | Pentadecanoic acid  | 242              | C15H30O2 | 001002-84-2 | 93   |
| 3       |          | Tetradecanoic acid  | 228              | C14H28O2 | 000544-63-8 | 91   |
| 4       |          | Tridecanoic acid    | 214              | C13H26O2 | 000638-53-9 | 81   |
| 5       |          | Undecane, 2-methyl- | 170              | C12H26   | 007045-71-8 | 25   |



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ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

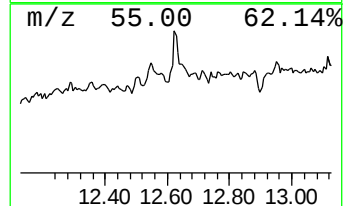
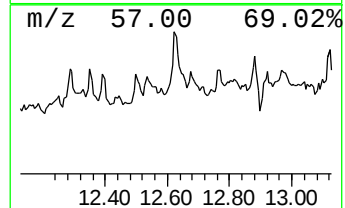
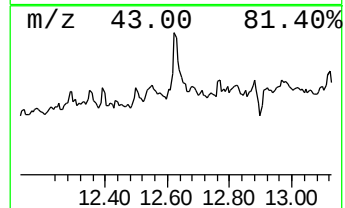
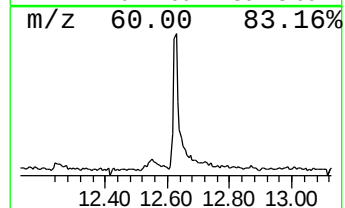
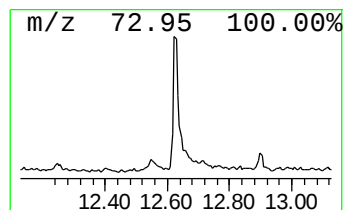
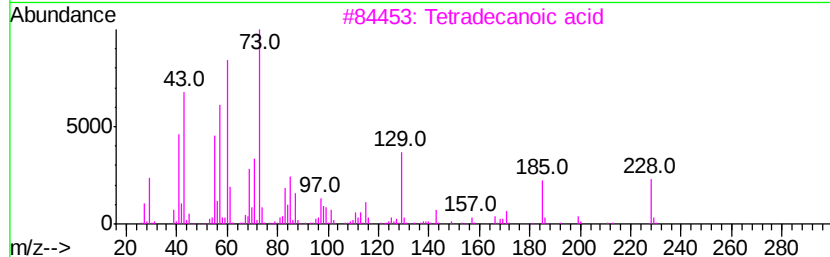
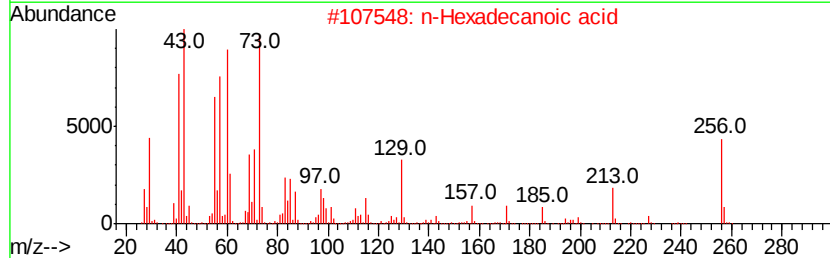
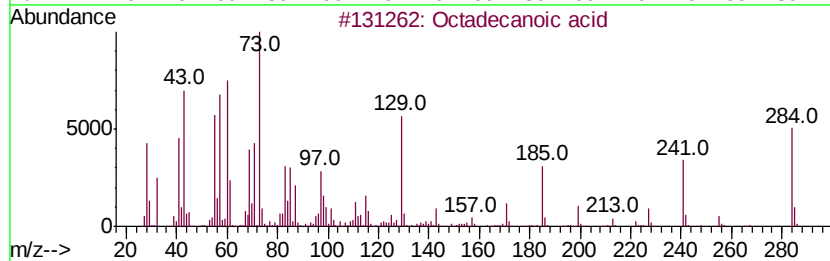
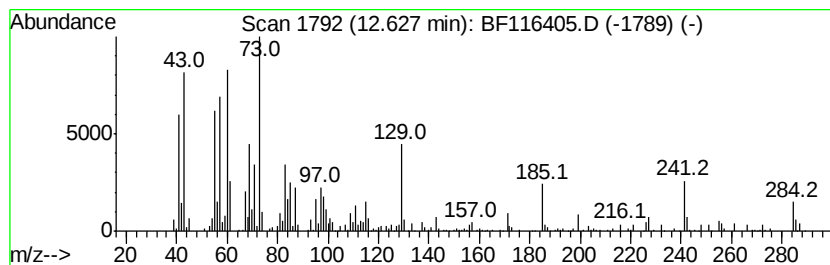
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octadecanoic acid Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.63 | 3.58 ng | 175767 | Phenanthrene-d10 | 11.32 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | Octadecanoic acid                    | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    | n-Hexadecanoic acid                  | 256 | C16H32O2 | 000057-10-3 | 93   |
| 3    |    | Tetradecanoic acid                   | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4    |    | Octadecanoic acid, 2-(2-hydroxyve... | 372 | C22H44O4 | 000106-11-6 | 80   |
| 5    |    | Pentadecanoic acid                   | 242 | C15H30O2 | 001002-84-2 | 70   |



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ALS Vial : 14 Sample Multiplier: 1

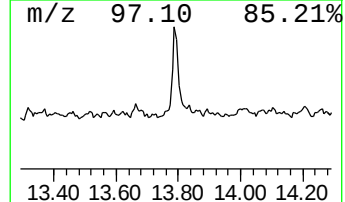
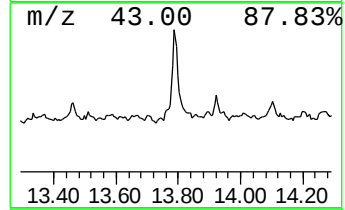
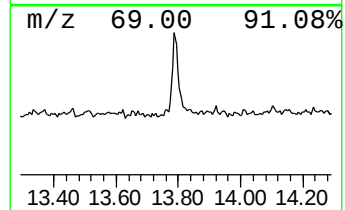
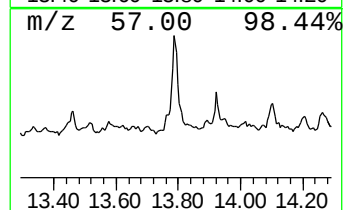
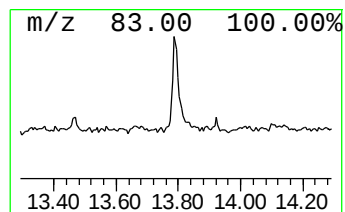
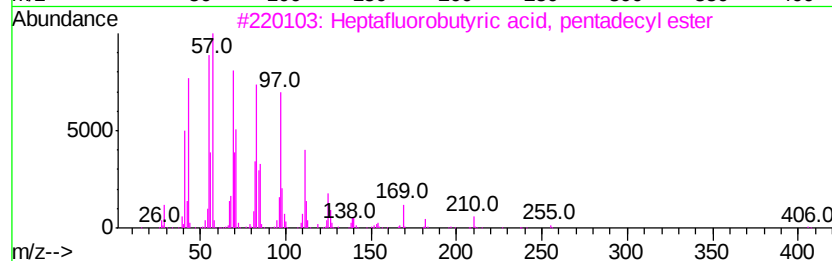
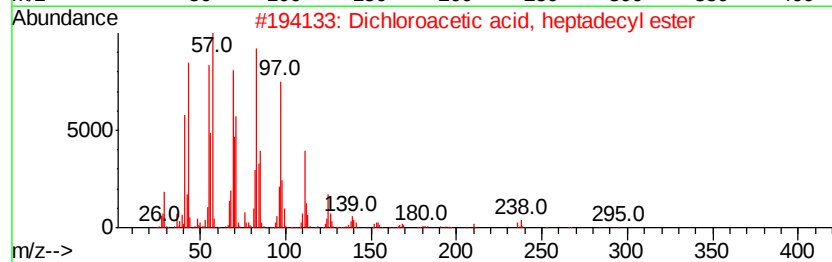
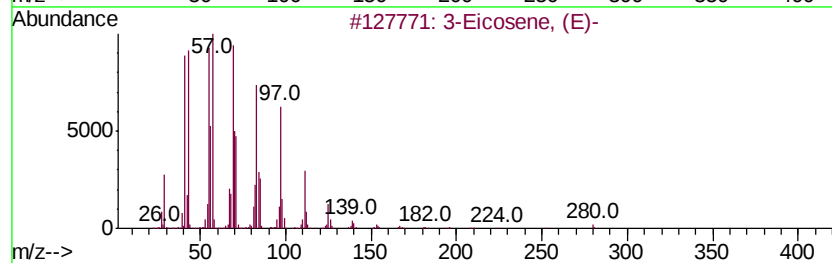
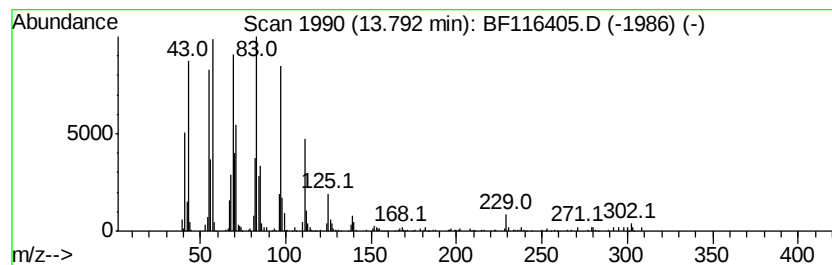
Instrument :  
BNA\_F  
ClientSampleId :  
B-2

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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 5 3-Eicosene, (E)- Concentration Rank 4

| R.T.    | EstConc | Area                                | Relative to ISTD | R.T.            |
|---------|---------|-------------------------------------|------------------|-----------------|
| 13.79   | 8.40 ng | 340040                              | Chrysene-d12     | 13.96           |
| Hit# of | 5       | Tentative ID                        | MW MolForm       | CAS# Qual       |
| 1       |         | 3-Eicosene, (E)-                    | 280 C20H40       | 074685-33-9 95  |
| 2       |         | Dichloroacetic acid, heptadecyl ... | 366 C19H36Cl2O2  | 1000282-98-2 94 |
| 3       |         | Heptafluorobutyric acid, pentade... | 424 C19H31F7O2   | 959261-23-5 93  |
| 4       |         | 2- Chloropropionic acid, octadec... | 360 C21H41ClO2   | 088104-31-8 91  |
| 5       |         | Heptadecyl heptafluorobutyrate      | 452 C21H35F7O2   | 959085-66-6 91  |



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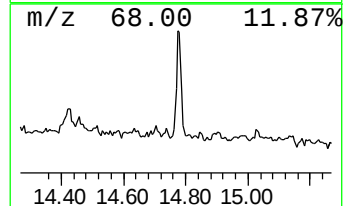
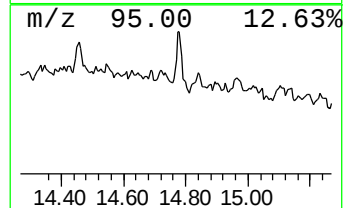
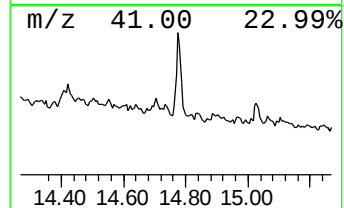
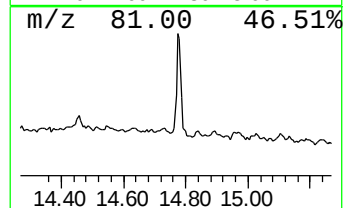
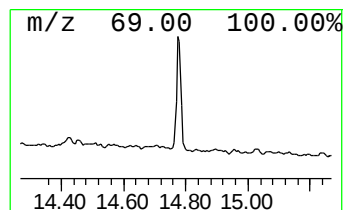
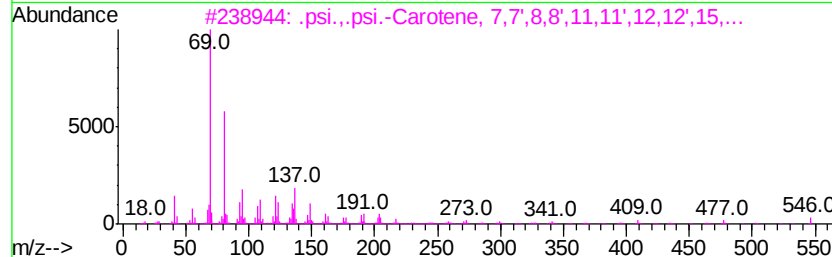
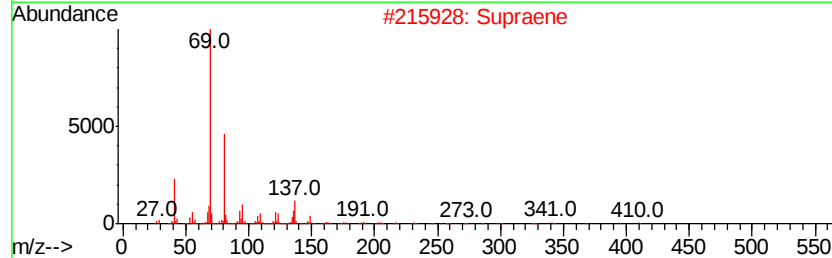
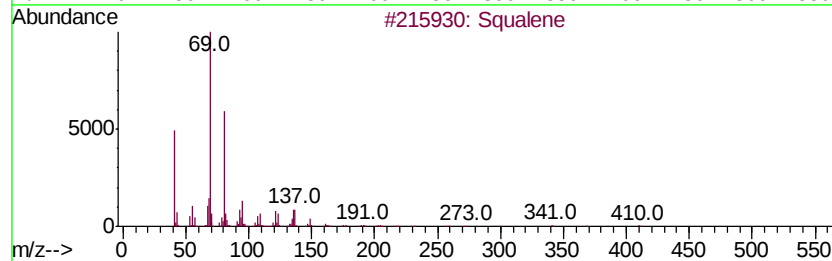
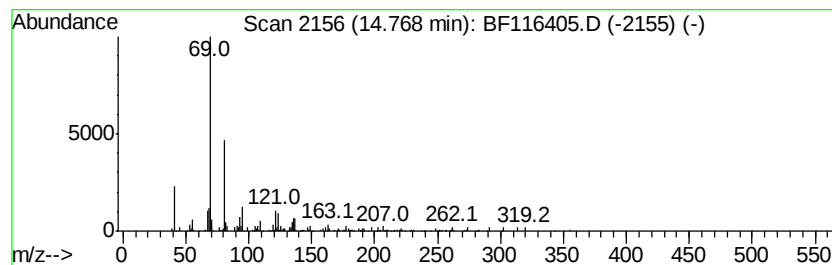
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Squalene Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.77 | 5.68 ng | 220925 | Perylene-d12     | 15.42 |

| Hit# | of | Tentative ID                         | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Squalene                             | 410 | C30H50  | 000111-02-4 | 91   |
| 2    |    | Supraene                             | 410 | C30H50  | 007683-64-9 | 90   |
| 3    |    | .psi.,.psi.-Carotene, 7,7',8,8',.... | 547 | C40H66  | 000502-62-5 | 83   |
| 4    |    | 4,9,13,17-Tetramethyl-4,8,12,16-...  | 316 | C22H36O | 056882-09-8 | 83   |
| 5    |    | 1,5,9-Undecatriene, 2,6,10-trime...  | 192 | C14H24  | 062951-96-6 | 72   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF081919\  
Data File : BF116405.D  
Acq On : 19 Aug 2019 23:17  
Operator : HP/JU  
Sample : K4290-02  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

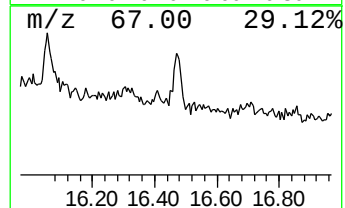
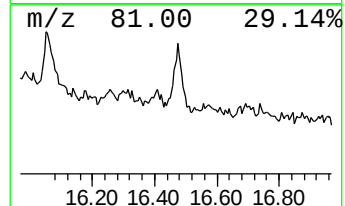
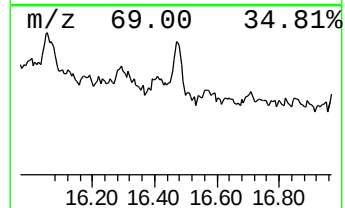
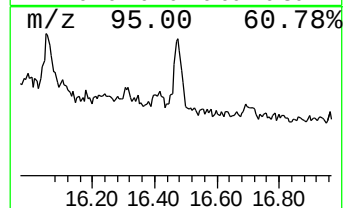
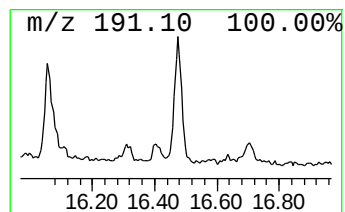
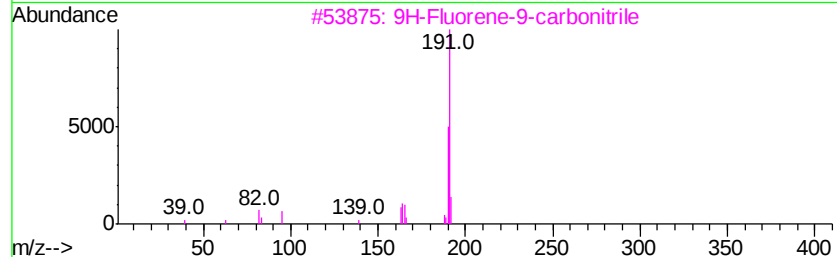
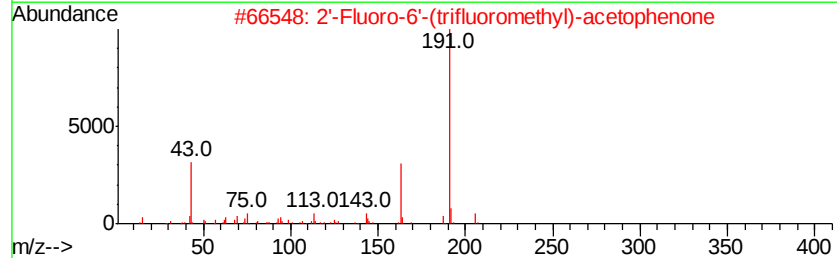
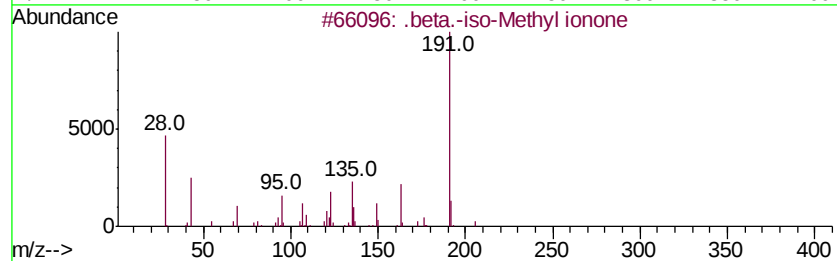
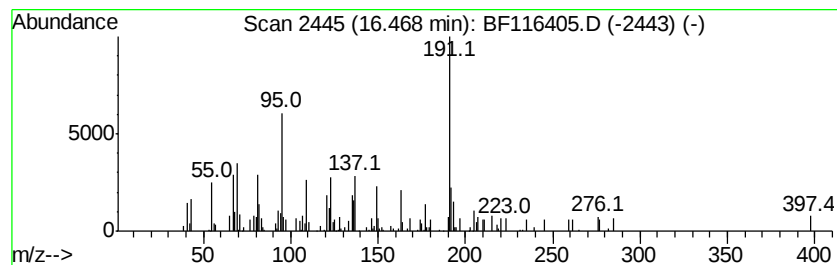
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 .beta.-iso-Methyl ionone Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.47 | 3.24 ng | 125845 | Perylene-d12     | 15.42 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | .beta.-iso-Methyl ionone            | 206 | C14H22O | 1000285-40-2 | 53   |
| 2    |    | 2'-Fluoro-6'-(trifluoromethyl)-a... | 206 | C9H6F4O | 174013-29-7  | 35   |
| 3    |    | 9H-Fluorene-9-carbonitrile          | 191 | C14H9N  | 001529-40-4  | 35   |
| 4    |    | 4H-Benzo[def]carbazole              | 191 | C14H9N  | 000203-65-6  | 35   |
| 5    |    | 5-(p-Aminophenyl)-2-thiazolamine    | 191 | C9H9N3S | 090349-87-4  | 35   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF081919\  
Data File : BF116405.D  
Acq On : 19 Aug 2019 23:17  
Operator : HP/JU  
Sample : K4290-02  
Misc :  
ALS Vial : 14 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
B-2

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF073019.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 |
| unknown6.58          | 6.58  | 85.4    | ng    | 2439540  | 1                     | 6.80  | 571552 | 20.0 |
| n-Hexadecanoic acid  | 11.85 | 13.1    | ng    | 639869   | 4                     | 11.32 | 980964 | 20.0 |
| Octadecanoic acid    | 12.63 | 3.6     | ng    | 175767   | 4                     | 11.32 | 980964 | 20.0 |
| 3-Eicosene, (E)-     | 13.79 | 8.4     | ng    | 340040   | 5                     | 13.96 | 809455 | 20.0 |
| Squalene             | 14.77 | 5.7     | ng    | 220925   | 6                     | 15.42 | 777433 | 20.0 |
| .beta.-iso-Methyl... | 16.47 | 3.2     | ng    | 125845   | 6                     | 15.42 | 777433 | 20.0 |