

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF060122\  
 Data File : BF128625.D  
 Acq On : 01 Jun 2022 16:25  
 Operator : CG\JU  
 Sample : N2953-10  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P044-SS001-1824-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128625.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         | 3.381       | 183           | 186         | 198          | rBV      | 20572          | 39625         | 1.52%           | 0.229%        |
| 2         | 5.057       | 466           | 471         | 477          | rVB      | 25171          | 33580         | 1.29%           | 0.194%        |
| 3         | 5.493       | 541           | 545         | 563          | rVB      | 2203240        | 2446954       | 94.03%          | 14.114%       |
| 4         | 6.504       | 714           | 717         | 727          | rBV      | 2302373        | 2477502       | 95.21%          | 14.290%       |
| 5         | 6.575       | 727           | 729         | 733          | rVB      | 63077          | 51404         | 1.98%           | 0.297%        |
| 6         | 6.834       | 769           | 773         | 776          | rBV      | 719501         | 562269        | 21.61%          | 3.243%        |
| 7         | 7.398       | 863           | 869         | 872          | rBV      | 1708894        | 1648946       | 63.37%          | 9.511%        |
| 8         | 8.116       | 987           | 991         | 994          | rBV      | 874198         | 712660        | 27.39%          | 4.111%        |
| 9         | 9.192       | 1169          | 1174        | 1177         | rBV      | 3228578        | 2602197       | 100.00%         | 15.010%       |
| 10        | 9.869       | 1285          | 1289        | 1292         | rBV      | 865276         | 667901        | 25.67%          | 3.853%        |
| 11        | 10.663      | 1420          | 1424        | 1427         | rBV      | 1740320        | 1454000       | 55.88%          | 8.387%        |
| 12        | 11.351      | 1538          | 1541        | 1545         | rBV      | 642975         | 597490        | 22.96%          | 3.446%        |
| 13        | 11.886      | 1628          | 1632        | 1645         | rBV      | 331632         | 347767        | 13.36%          | 2.006%        |
| 14        | 12.592      | 1747          | 1752        | 1760         | rBV      | 56472          | 81919         | 3.15%           | 0.473%        |
| 15        | 12.674      | 1762          | 1766        | 1777         | rVV      | 176932         | 194974        | 7.49%           | 1.125%        |
| 16        | 12.945      | 1807          | 1812        | 1815         | rBV      | 2154449        | 1940283       | 74.56%          | 11.192%       |
| 17        | 13.916      | 1971          | 1977        | 1985         | rBV3     | 48103          | 126317        | 4.85%           | 0.729%        |
| 18        | 13.992      | 1985          | 1990        | 1994         | rVB      | 577693         | 551573        | 21.20%          | 3.182%        |
| 19        | 14.092      | 2002          | 2007        | 2012         | rBV      | 272137         | 265723        | 10.21%          | 1.533%        |
| 20        | 15.463      | 2235          | 2240        | 2244         | rBV      | 434549         | 533712        | 20.51%          | 3.078%        |

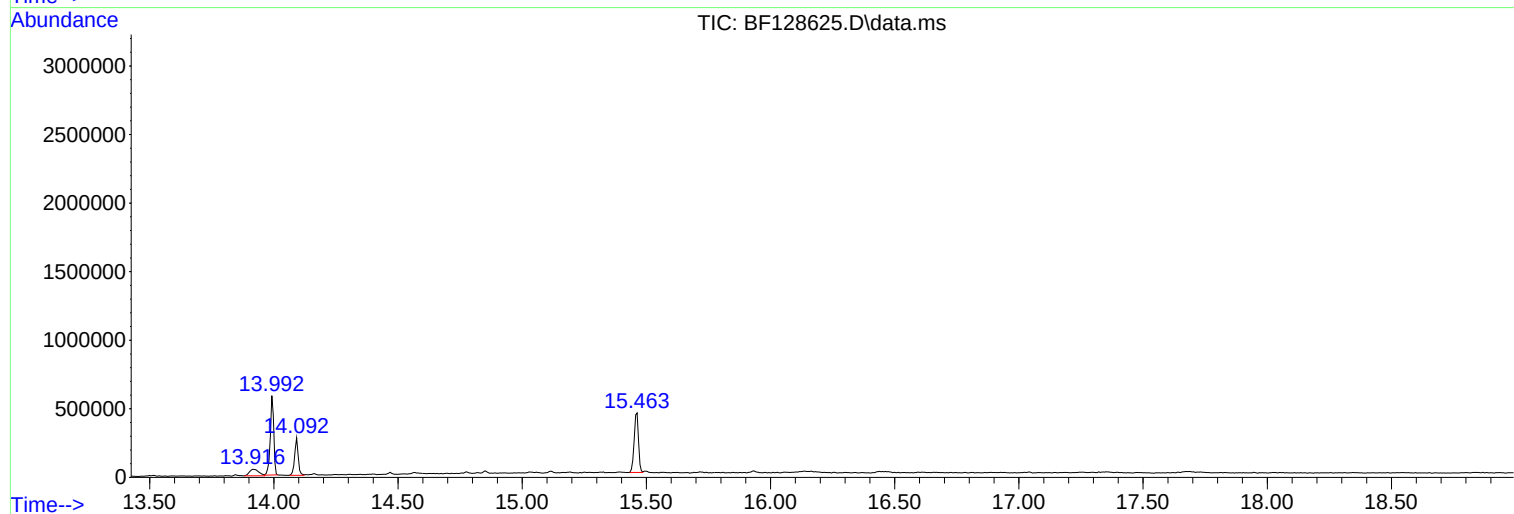
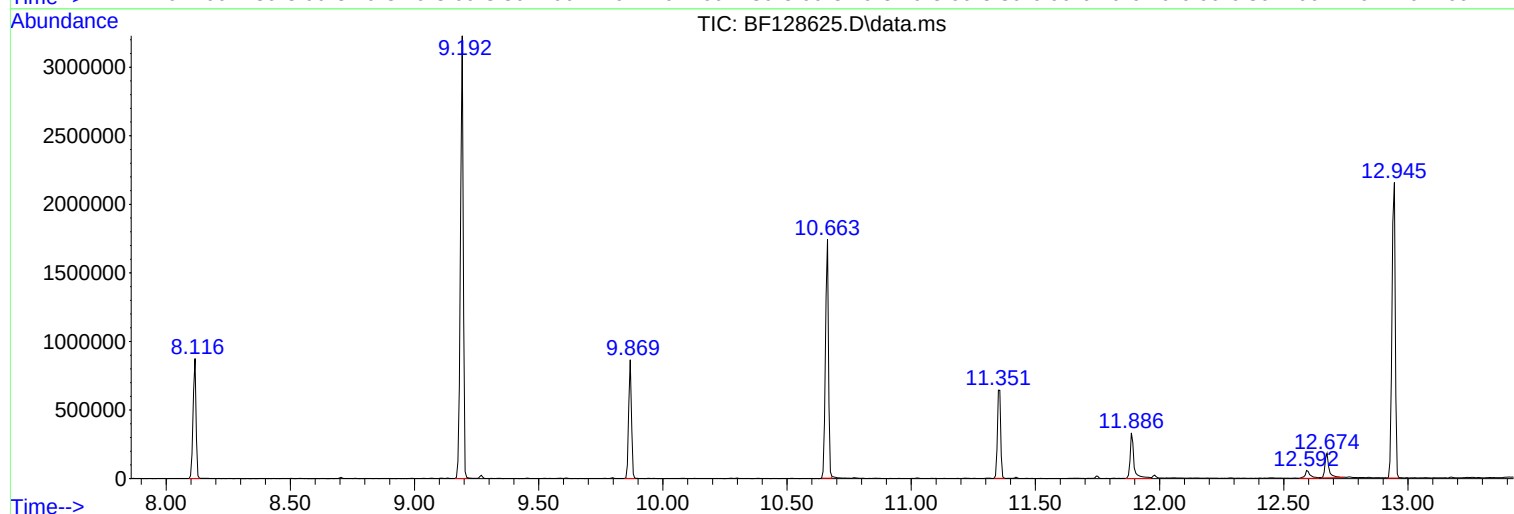
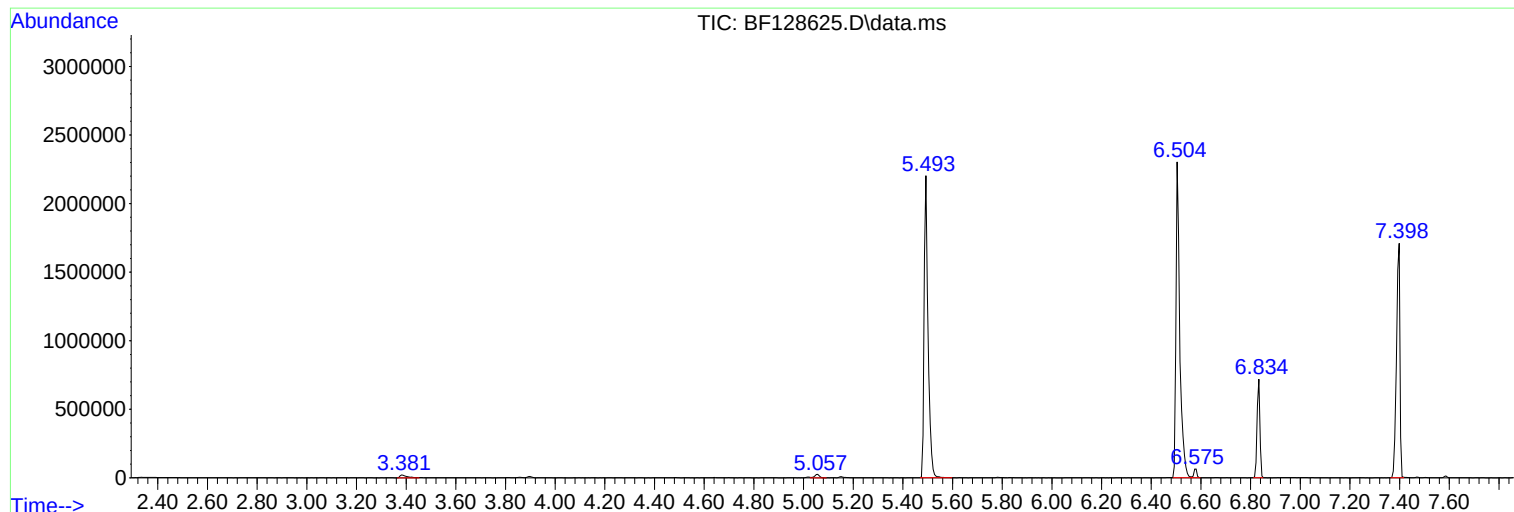
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Sample : N2953-10  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P044-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.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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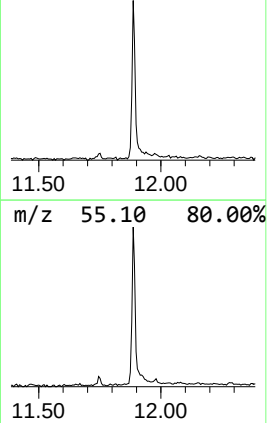
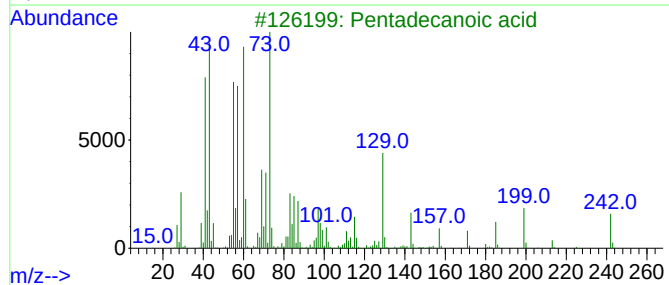
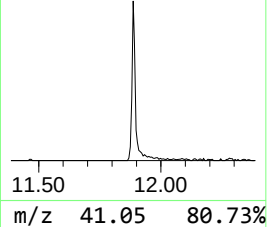
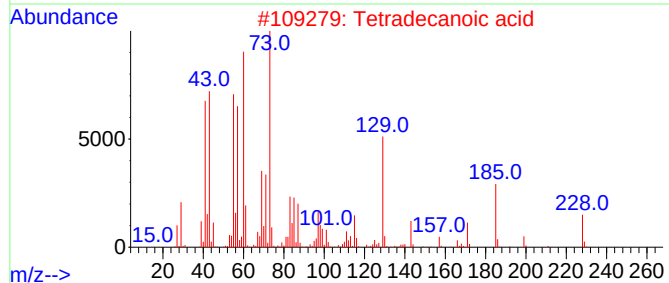
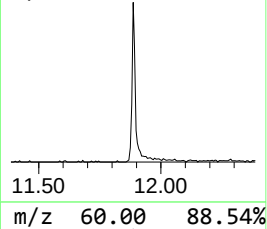
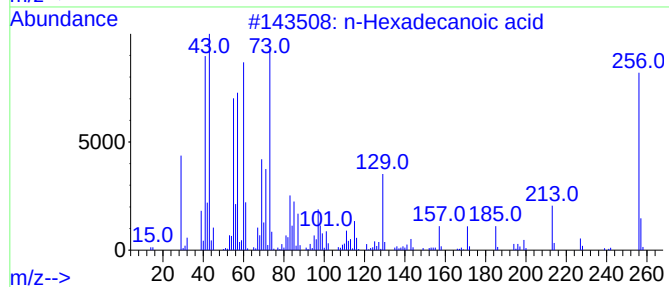
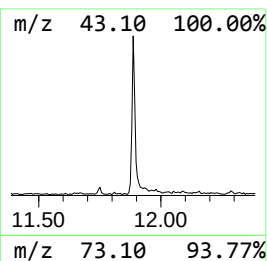
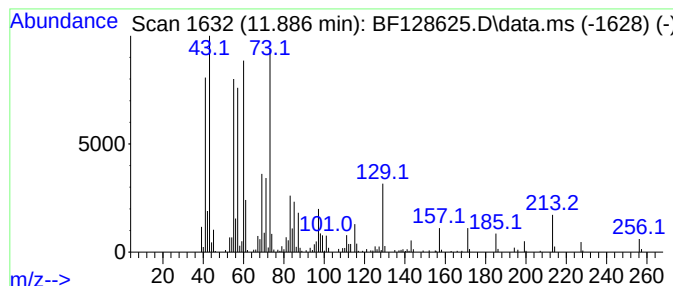
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 11.886 | 11.64 ng | 347767 | Phenanthrene-d10 | 11.357 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 91   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 81   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 59   |



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Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P044-SS001-1824-01

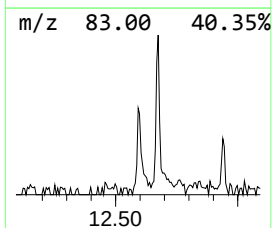
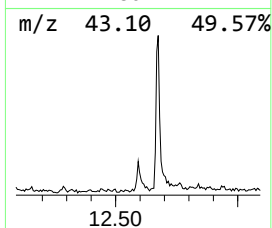
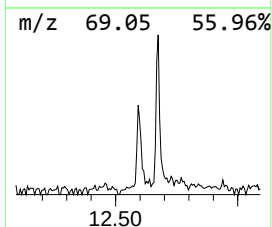
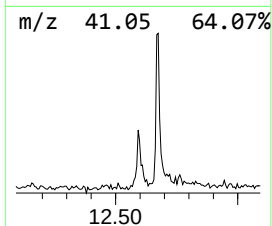
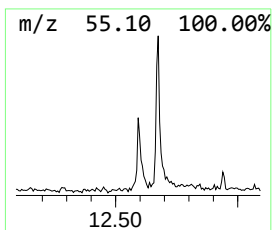
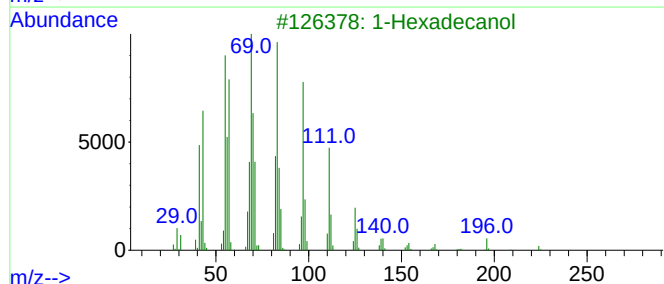
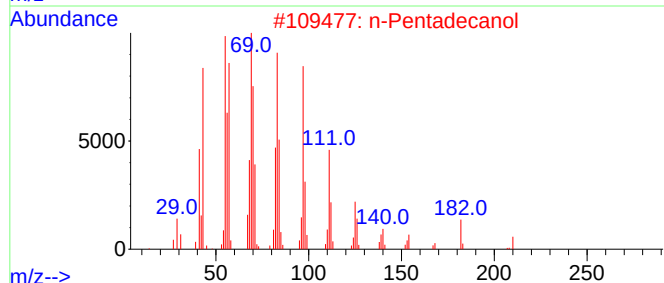
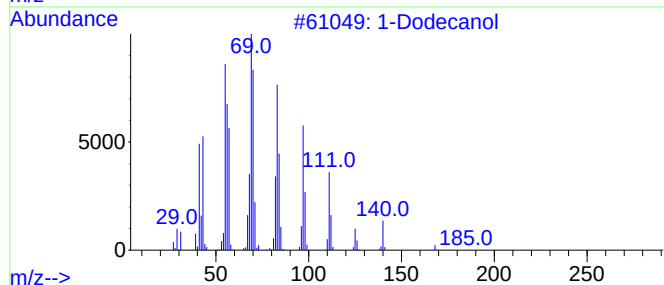
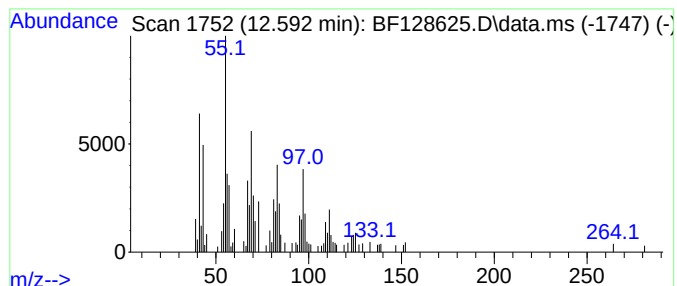
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 1-Dodecanol Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.592 | 2.74 ng | 81919 | Phenanthrene-d10 | 11.357 |

| Hit# | of 5 | Tentative ID             | MW  | MolForm  | CAS#        | Qual |
|------|------|--------------------------|-----|----------|-------------|------|
| 1    |      | 1-Dodecanol              | 186 | C12H26O  | 000112-53-8 | 64   |
| 2    |      | n-Pentadecanol           | 228 | C15H32O  | 000629-76-5 | 64   |
| 3    |      | 1-Hexadecanol            | 242 | C16H34O  | 036653-82-4 | 58   |
| 4    |      | Cyclohexadecane          | 224 | C16H32   | 000295-65-8 | 58   |
| 5    |      | cis-13-Octadecenoic acid | 282 | C18H34O2 | 013126-39-1 | 53   |



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ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P044-SS001-1824-01

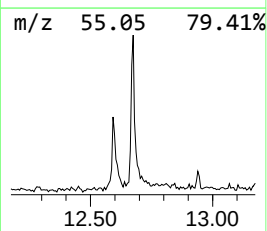
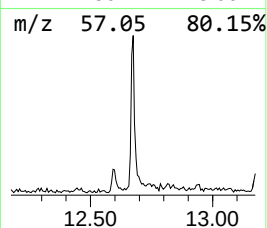
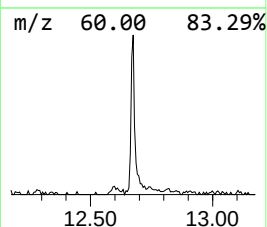
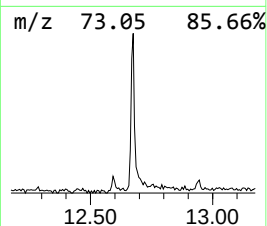
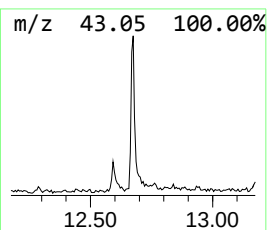
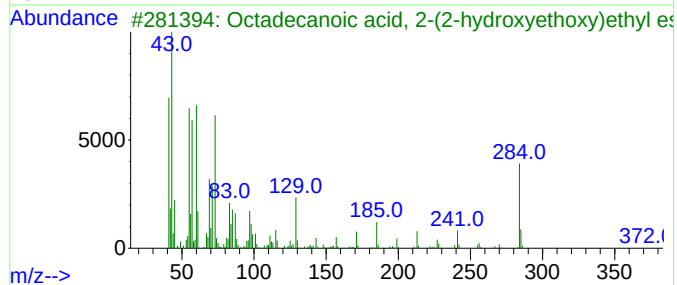
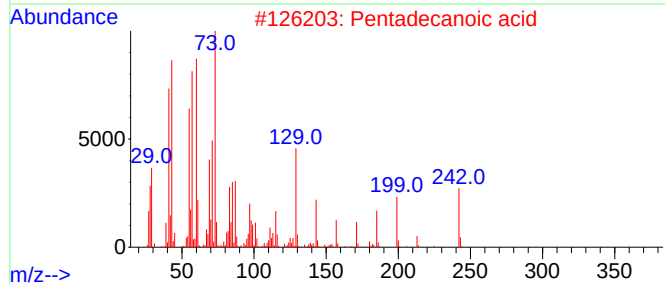
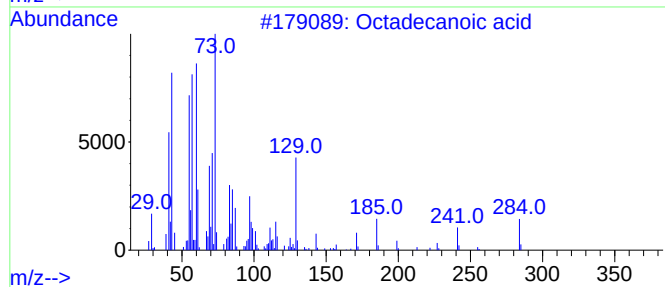
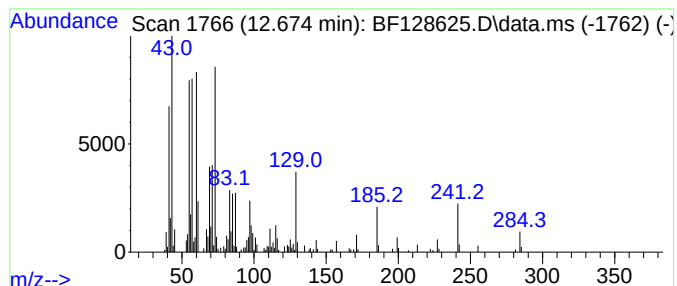
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.675 | 6.53 ng | 194974 | Phenanthrene-d10 | 11.357 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 90   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | 8-Methylnonanoic acid               | 172 | C10H20O2 | 005963-14-4 | 60   |



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Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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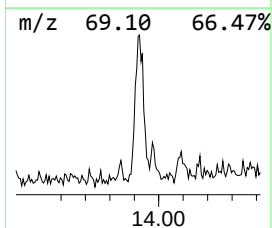
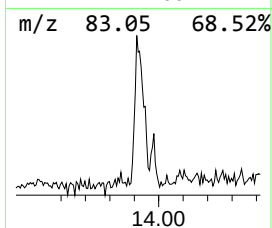
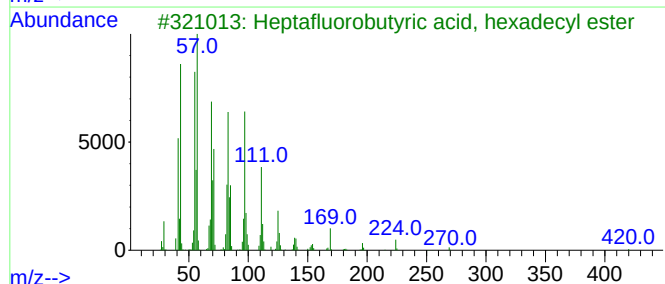
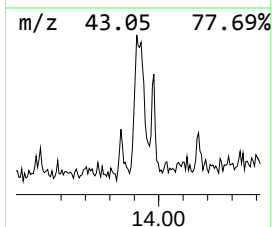
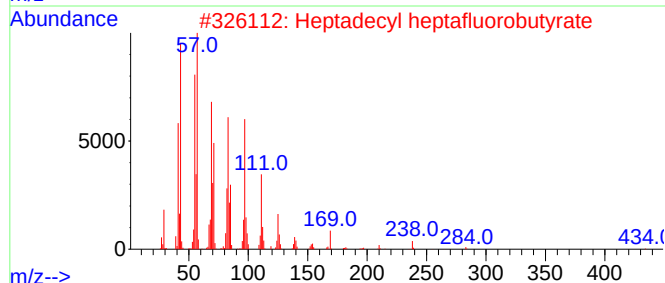
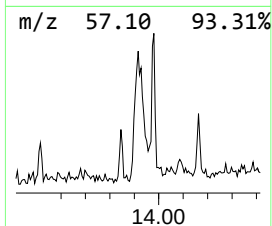
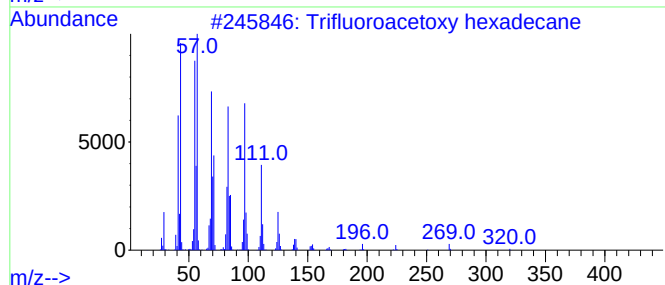
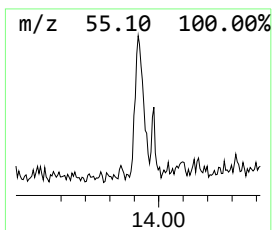
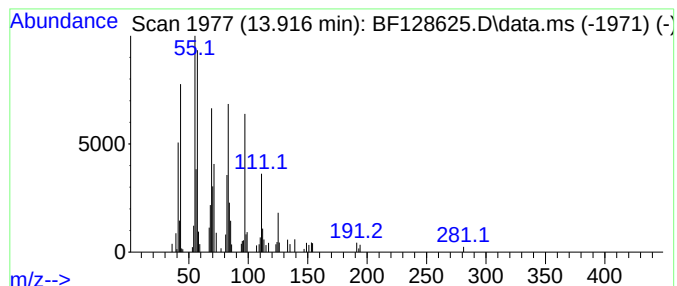
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.916 | 4.58 ng | 126317 | Chrysene-d12     | 13.992 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3 | 90   |
| 2    |    |   | Heptadecyl heptafluorobutyrate      | 452 | C21H35F7O2 | 959085-66-6 | 90   |
| 3    |    |   | Heptafluorobutyric acid, hexadec... | 438 | C20H33F7O2 | 006385-15-5 | 87   |
| 4    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 87   |
| 5    |    |   | Bromoacetic acid, octadecyl ester   | 390 | C20H39BrO2 | 018992-03-5 | 87   |



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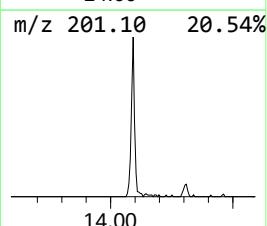
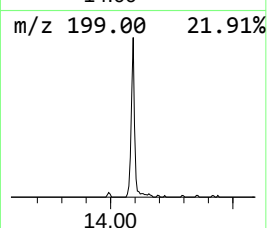
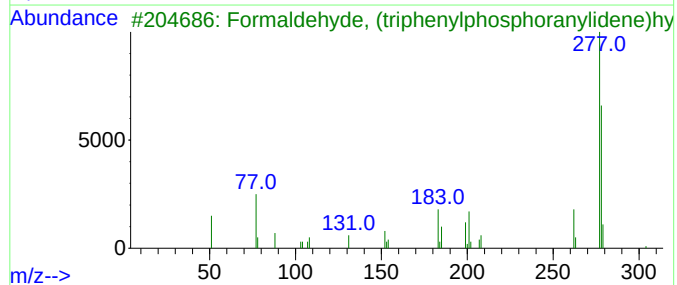
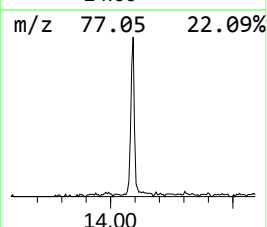
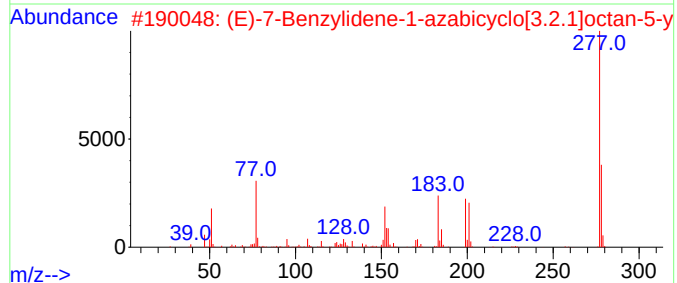
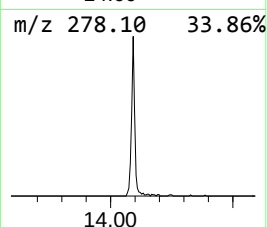
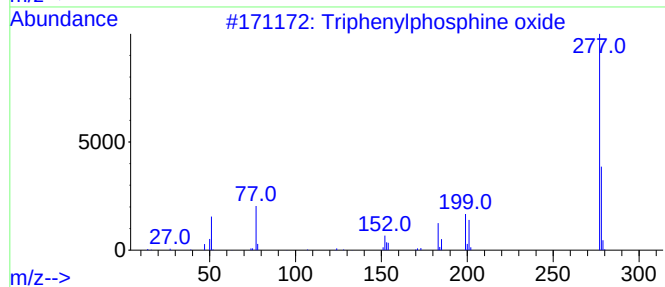
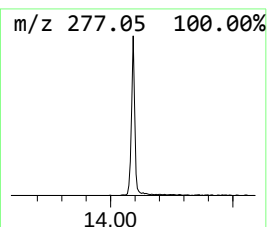
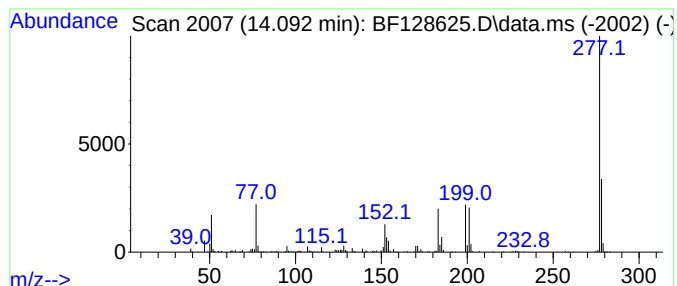
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Triphenylphosphine oxide Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.092 | 9.64 ng | 265723 | Chrysene-d12     | 13.992 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 97   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S | 1000483-83-4 | 64   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...] | 304 | C19H17N2P  | 015990-54-2  | 50   |
| 4    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd...  | 277 | C18H15N02  | 299962-12-2  | 37   |
| 5    |    |   | 2-Propenoic acid, 2-cyano-3-(3-p...  | 277 | C18H15N02  | 1000080-00-3 | 25   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF060122\  
Data File : BF128625.D  
Acq On : 01 Jun 2022 16:25  
Operator : CG\JU  
Sample : N2953-10  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P044-SS001-1824-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.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 ... | 11.886 | 11.6    | ng    | 347767   | 4                     | 11.357 | 597490 | 20.0 |
| 1-Dodecanol        | 12.592 | 2.7     | ng    | 81919    | 4                     | 11.357 | 597490 | 20.0 |
| Octadecanoic acid  | 12.675 | 6.5     | ng    | 194974   | 4                     | 11.357 | 597490 | 20.0 |
| Trifluoroacetox... | 13.916 | 4.6     | ng    | 126317   | 5                     | 13.992 | 551573 | 20.0 |
| Triphenylphosph... | 14.092 | 9.6     | ng    | 265723   | 5                     | 13.992 | 551573 | 20.0 |