

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122123\  
 Data File : BF136665.D  
 Acq On : 21 Dec 2023 12:11  
 Operator : CG\JU  
 Sample : 05585-02  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P3874-SP2

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-BF122023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136665.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         | 5.416       | 562           | 566         | 576          | rBV      | 1024289        | 877049        | 34.09%          | 6.641%        |
| 2         | 6.416       | 732           | 736         | 747          | rBV      | 620789         | 532302        | 20.69%          | 4.030%        |
| 3         | 6.781       | 794           | 798         | 801          | rBV      | 468651         | 414090        | 16.09%          | 3.135%        |
| 4         | 7.345       | 888           | 894         | 896          | rBV      | 1290780        | 1364544       | 53.03%          | 10.332%       |
| 5         | 8.057       | 1010          | 1015        | 1018         | rBV      | 611238         | 543240        | 21.11%          | 4.113%        |
| 6         | 9.139       | 1193          | 1199        | 1201         | rBV      | 2590665        | 2573047       | 100.00%         | 19.483%       |
| 7         | 9.810       | 1309          | 1313        | 1317         | rBV      | 751279         | 616528        | 23.96%          | 4.668%        |
| 8         | 10.604      | 1444          | 1448        | 1452         | rBV      | 1436749        | 1485992       | 57.75%          | 11.252%       |
| 9         | 11.304      | 1563          | 1567        | 1570         | rBV      | 774395         | 642189        | 24.96%          | 4.863%        |
| 10        | 11.839      | 1652          | 1658        | 1674         | rBV      | 201838         | 282434        | 10.98%          | 2.139%        |
| 11        | 12.033      | 1680          | 1691        | 1693         | rBV4     | 23660          | 60619         | 2.36%           | 0.459%        |
| 12        | 12.627      | 1787          | 1792        | 1801         | rBV      | 150566         | 197513        | 7.68%           | 1.496%        |
| 13        | 12.904      | 1834          | 1839        | 1842         | rBV      | 2441489        | 2320905       | 90.20%          | 17.573%       |
| 14        | 13.268      | 1892          | 1901        | 1911         | rBV2     | 60433          | 145579        | 5.66%           | 1.102%        |
| 15        | 13.951      | 2013          | 2017        | 2021         | rBV      | 425012         | 416388        | 16.18%          | 3.153%        |
| 16        | 14.021      | 2023          | 2029        | 2041         | rVV2     | 54660          | 134167        | 5.21%           | 1.016%        |
| 17        | 14.598      | 2121          | 2127        | 2135         | rBV      | 53825          | 98229         | 3.82%           | 0.744%        |
| 18        | 15.198      | 2221          | 2229        | 2234         | rBV2     | 28999          | 61798         | 2.40%           | 0.468%        |
| 19        | 15.427      | 2263          | 2268        | 2273         | rBV      | 318113         | 375210        | 14.58%          | 2.841%        |
| 20        | 15.874      | 2338          | 2344        | 2348         | rBV3     | 17206          | 39067         | 1.52%           | 0.296%        |
| 21        | 16.662      | 2473          | 2478        | 2486         | rVB8     | 10870          | 25986         | 1.01%           | 0.197%        |

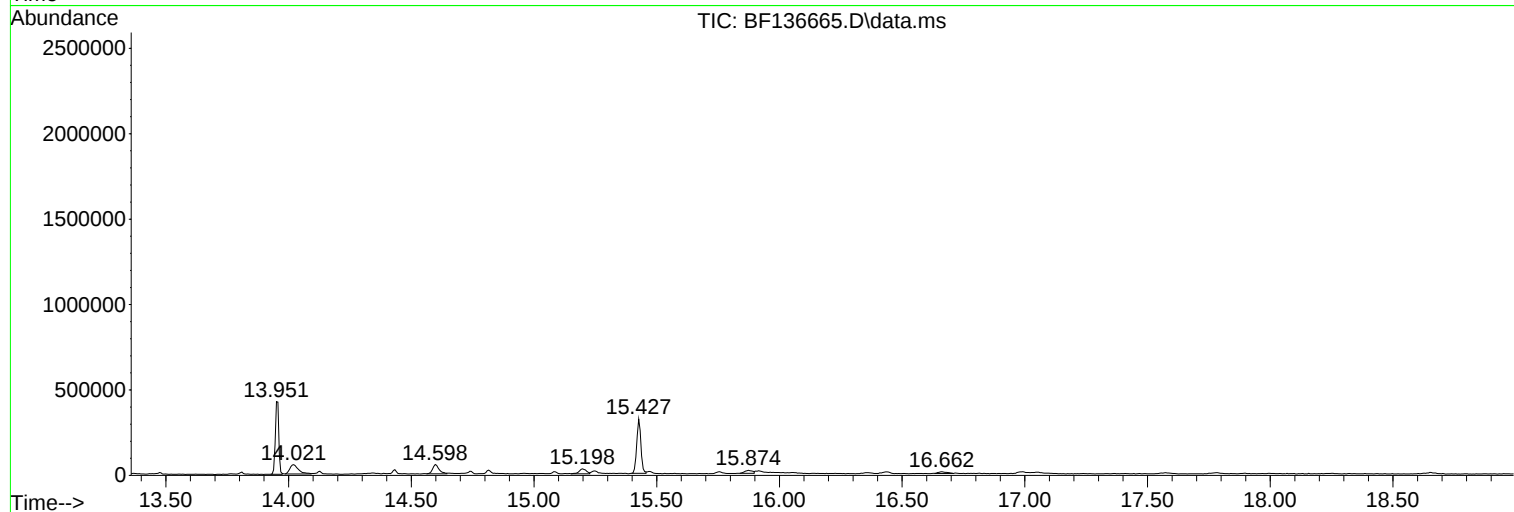
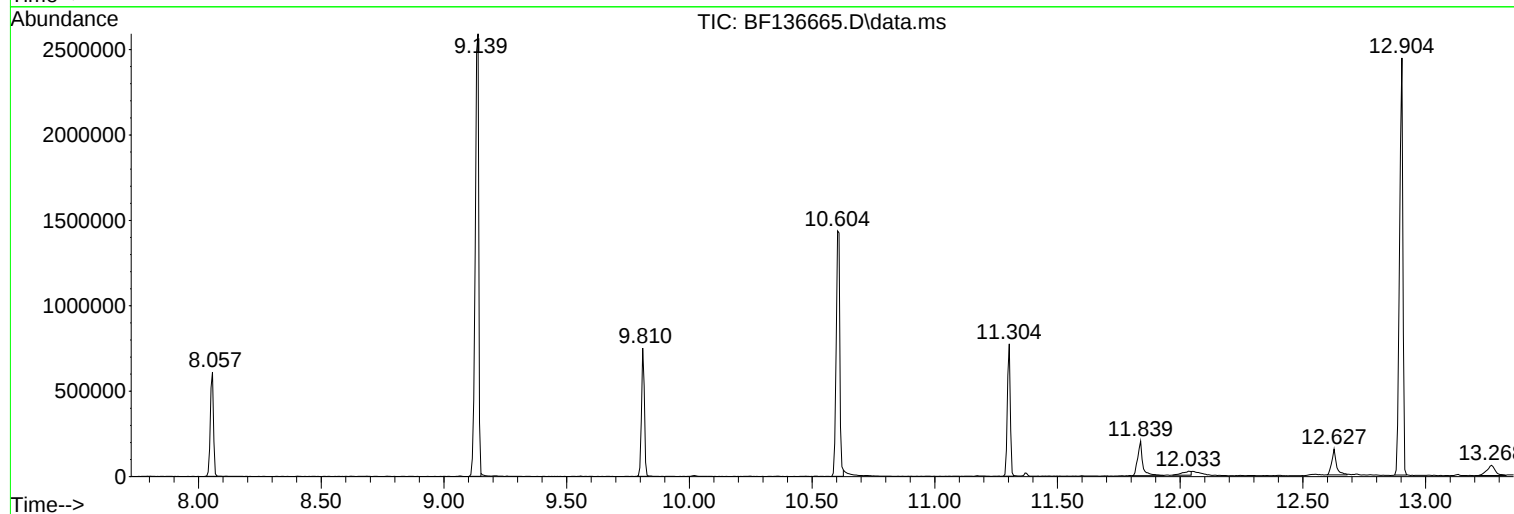
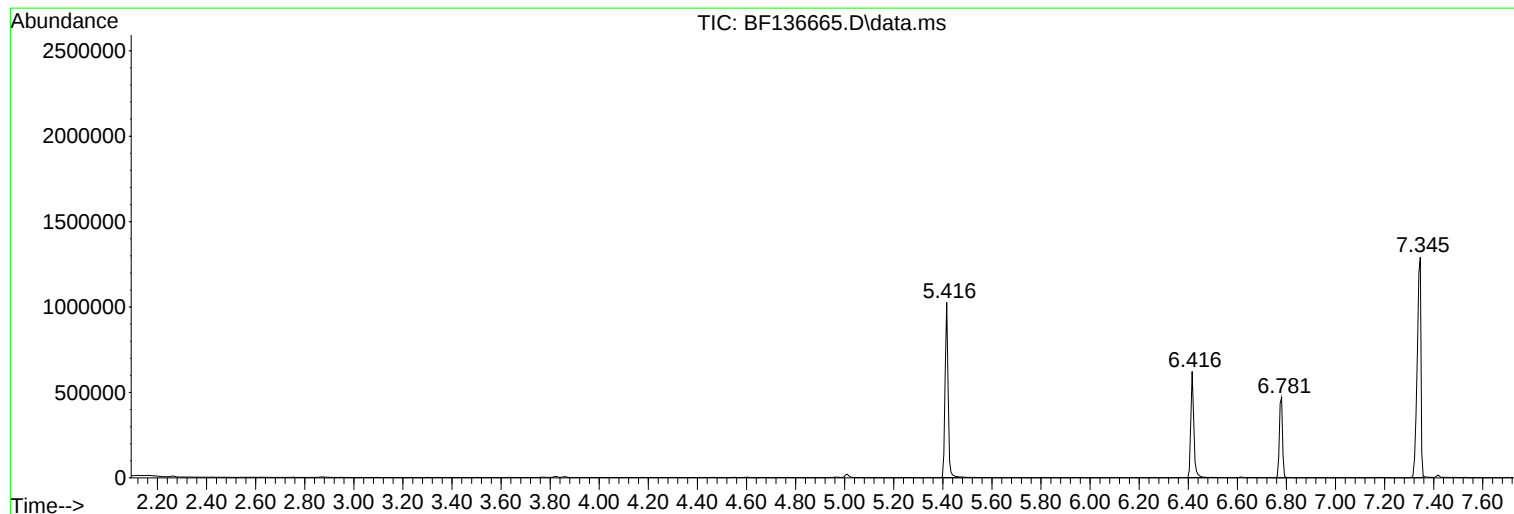
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Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122123\  
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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.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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Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

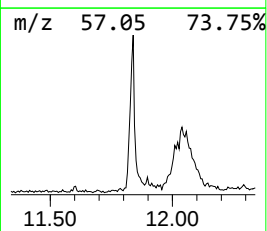
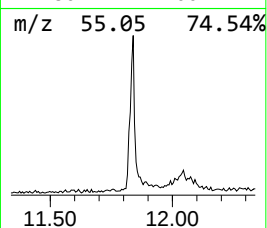
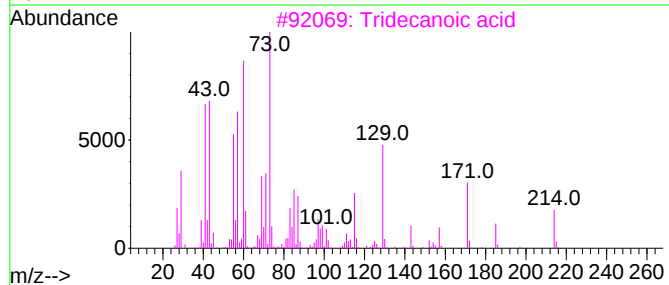
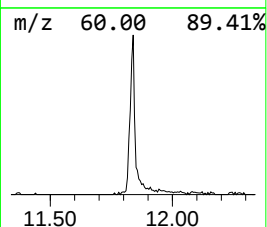
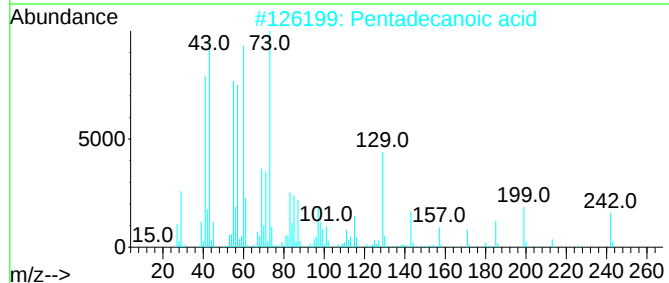
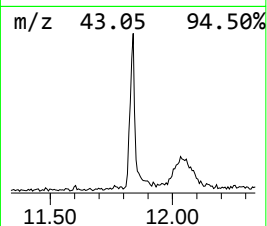
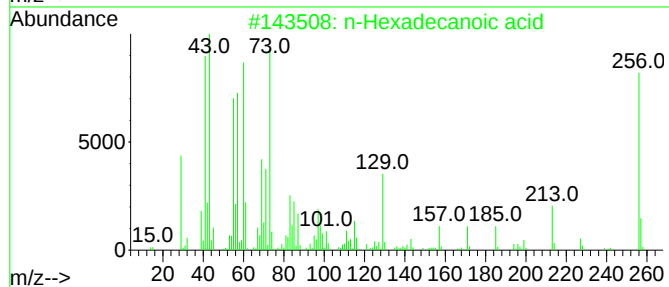
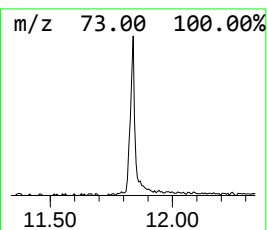
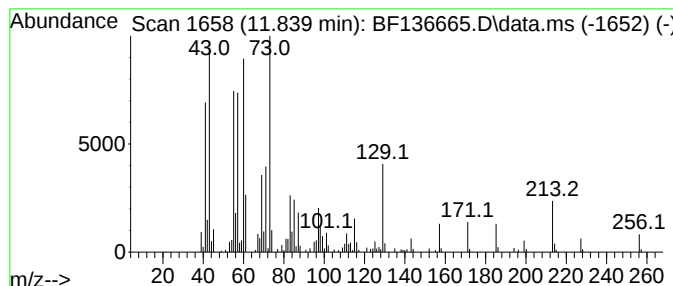
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.839 | 8.80 ng | 282434 | Phenanthrene-d10 | 11.304 |

| 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 | 93   |
| 3    |    |   | Tridecanoic acid      | 214 | C13H26O2 | 000638-53-9 | 92   |
| 4    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 90   |
| 5    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 70   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

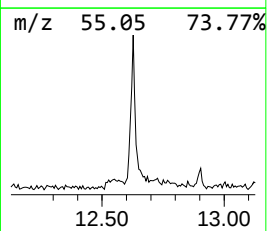
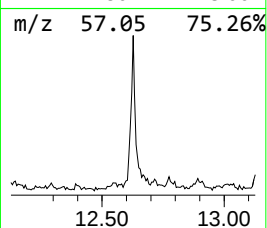
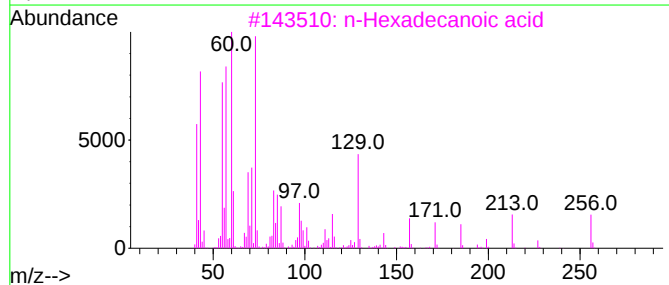
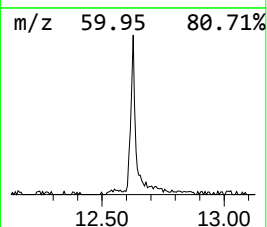
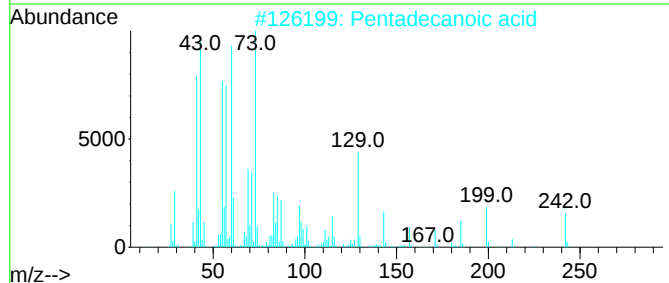
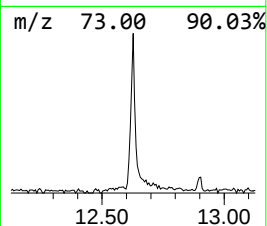
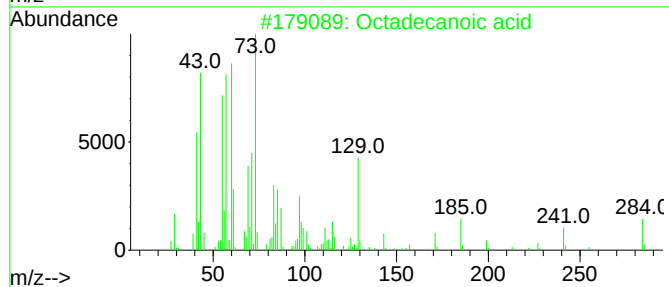
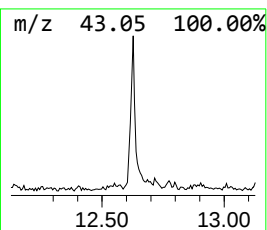
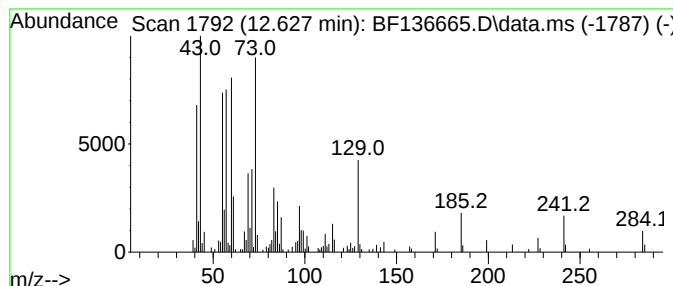
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Octadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.627 | 6.15 ng | 197513 | Phenanthrene-d10 | 11.304 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 70   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122123\  
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Sample : 05585-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

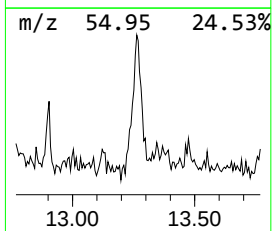
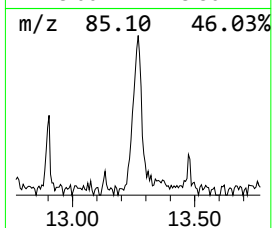
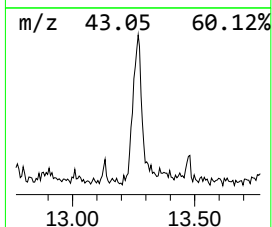
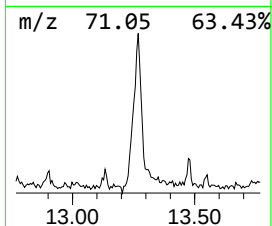
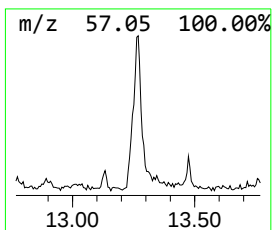
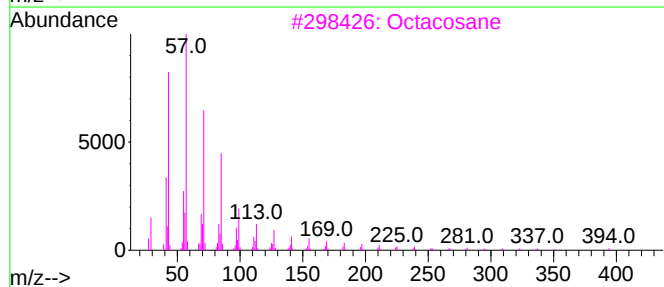
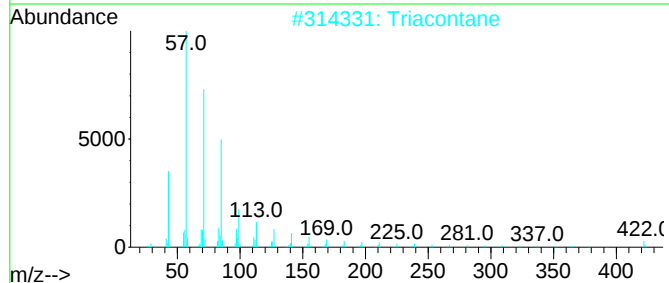
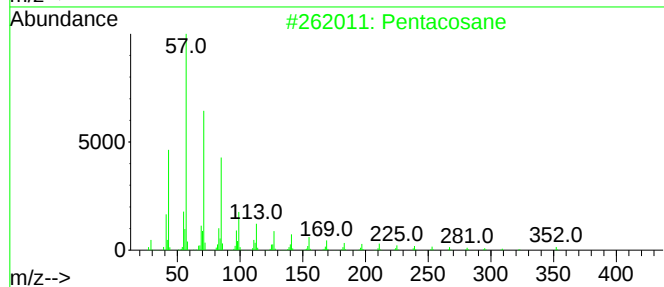
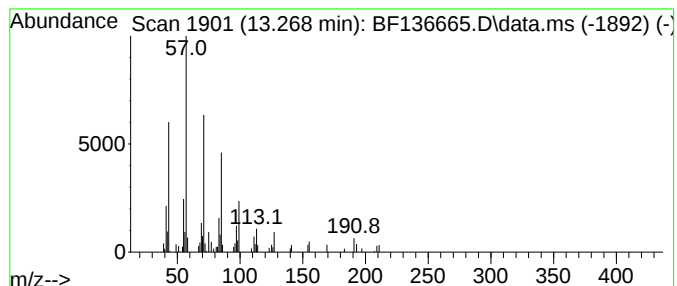
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Pentacosane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.268 | 6.99 ng | 145579 | Chrysene-d12     | 13.957 |

| Hit# | of | 5 | Tentative ID   | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------|-----|---------|-------------|------|
| 1    |    |   | Pentacosane    | 352 | C25H52  | 000629-99-2 | 83   |
| 2    |    |   | Triacontane    | 422 | C30H62  | 000638-68-6 | 80   |
| 3    |    |   | Octacosane     | 394 | C28H58  | 000630-02-4 | 80   |
| 4    |    |   | Hentriacontane | 437 | C31H64  | 000630-04-6 | 80   |
| 5    |    |   | Octadecane     | 254 | C18H38  | 000593-45-3 | 72   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

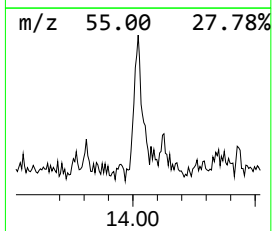
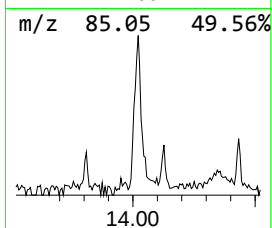
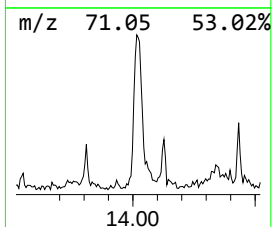
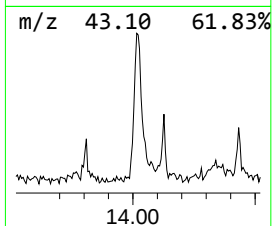
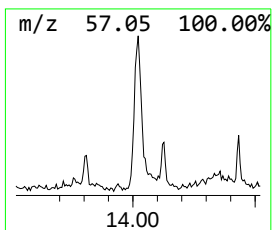
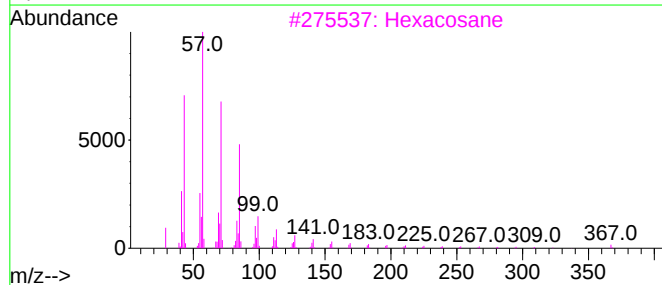
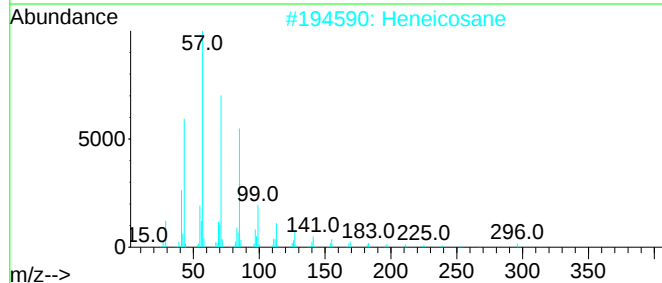
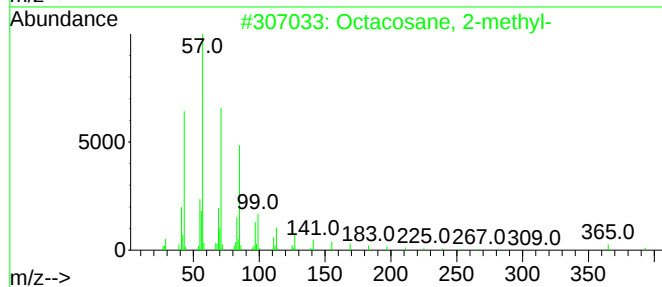
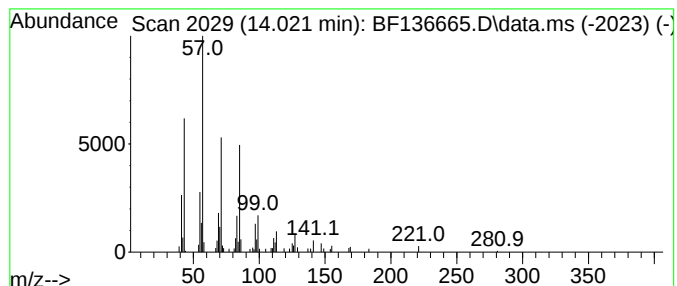
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 4 Octacosane, 2-methyl- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.021 | 6.44 ng | 134167 | Chrysene-d12     | 13.957 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|------|-------------------------------------|-----|-----------|--------------|------|
| 1    |      | Octacosane, 2-methyl-               | 408 | C29H60    | 001560-98-1  | 91   |
| 2    |      | Heneicosane                         | 296 | C21H44    | 000629-94-7  | 87   |
| 3    |      | Hexacosane                          | 366 | C26H54    | 000630-01-3  | 87   |
| 4    |      | Heptadecane, 9-octyl-               | 352 | C25H52    | 007225-64-1  | 87   |
| 5    |      | Sulfurous acid, 2-propyl tridecy... | 306 | C16H34O3S | 1000309-12-4 | 87   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

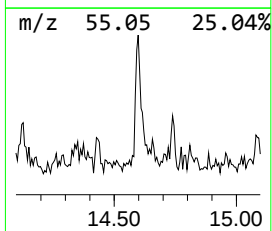
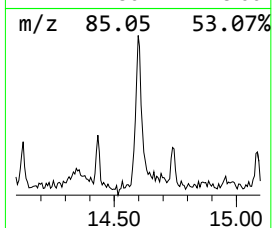
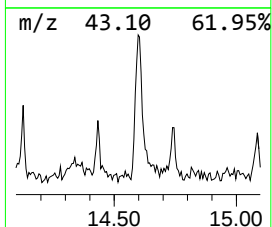
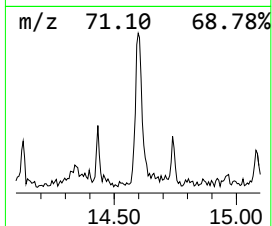
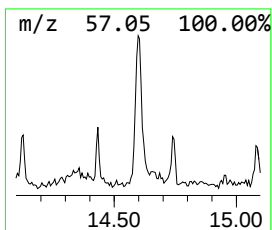
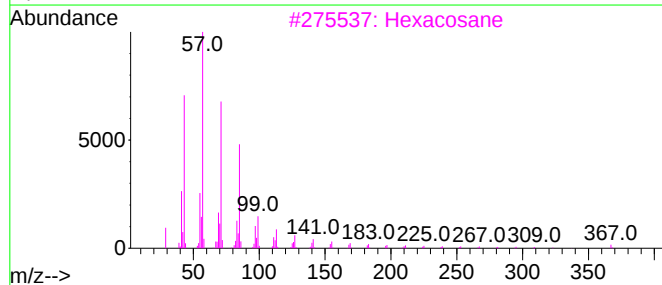
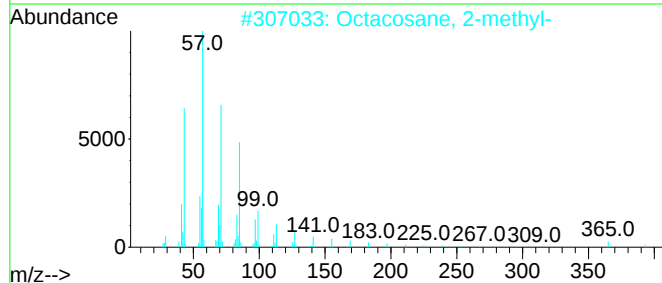
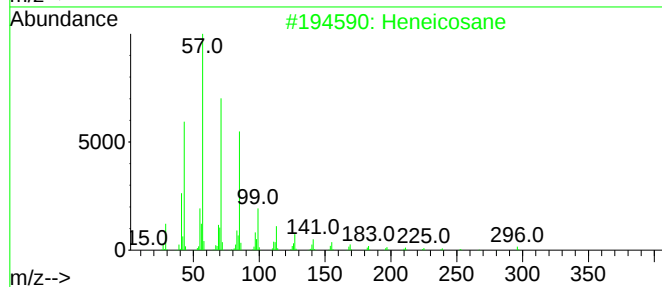
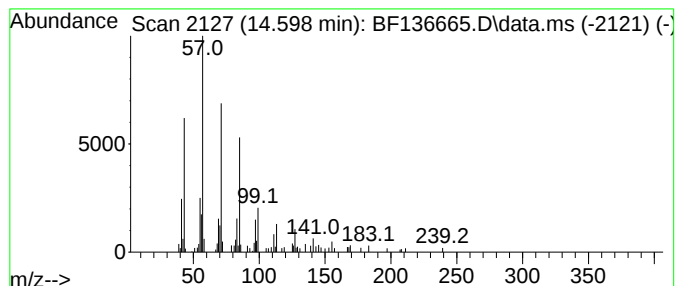
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Heneicosane Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.598 | 4.72 ng | 98229 | Chrysene-d12     | 13.957 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm  | CAS#        | Qual |
|------|----|---|----------------------------------|-----|----------|-------------|------|
| 1    |    |   | Heneicosane                      | 296 | C21H44   | 000629-94-7 | 91   |
| 2    |    |   | Octacosane, 2-methyl-            | 408 | C29H60   | 001560-98-1 | 91   |
| 3    |    |   | Hexacosane                       | 366 | C26H54   | 000630-01-3 | 91   |
| 4    |    |   | Pentadecane, 7-(bromomethyl)-    | 304 | C16H33Br | 052997-43-0 | 91   |
| 5    |    |   | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54   | 055282-11-6 | 91   |



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Data File : BF136665.D  
Acq On : 21 Dec 2023 12:11  
Operator : CG\JU  
Sample : 05585-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

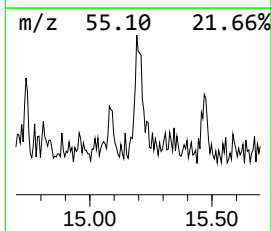
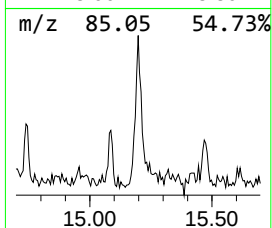
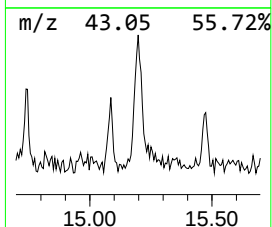
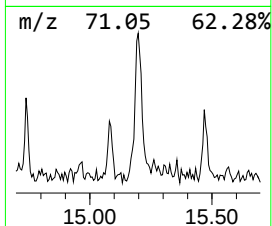
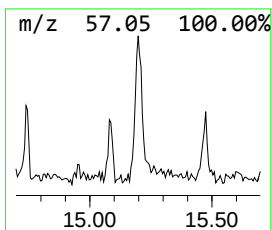
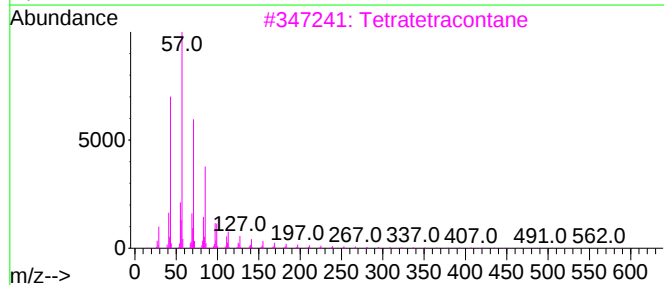
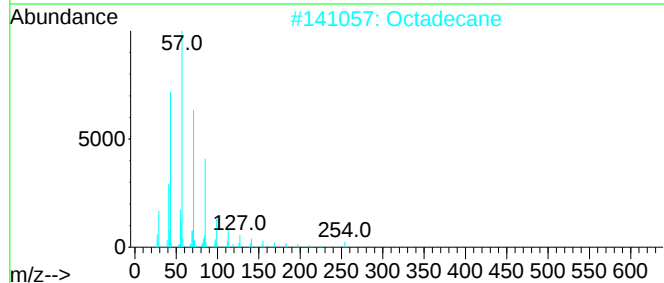
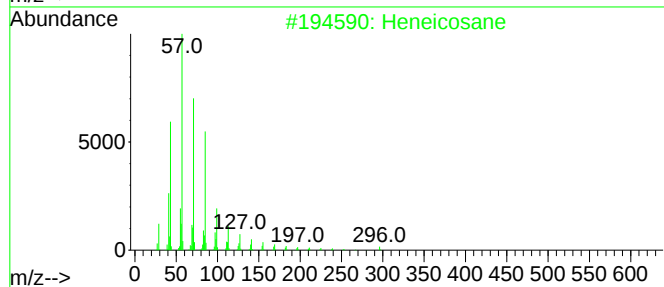
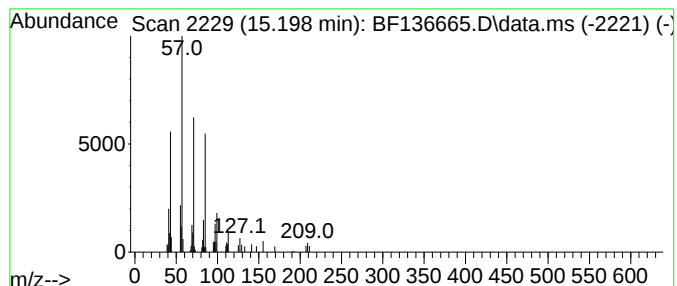
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Octadecane Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.198 | 3.29 ng | 61798 | Perylene-d12     | 15.427 |

| Hit# | of 5 | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|------|-------------------|-----|---------|-------------|------|
| 1    |      | Heneicosane       | 296 | C21H44  | 000629-94-7 | 87   |
| 2    |      | Octadecane        | 254 | C18H38  | 000593-45-3 | 78   |
| 3    |      | Tetratetracontane | 619 | C44H90  | 007098-22-8 | 74   |
| 4    |      | Heptacosane       | 380 | C27H56  | 000593-49-7 | 74   |
| 5    |      | Hexacosane        | 366 | C26H54  | 000630-01-3 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122123\  
Data File : BF136665.D  
Acq On : 21 Dec 2023 12:11  
Operator : CG\JU  
Sample : 05585-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

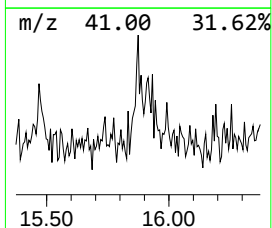
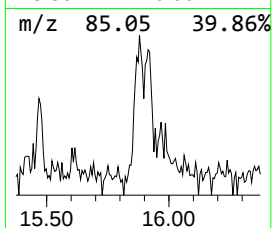
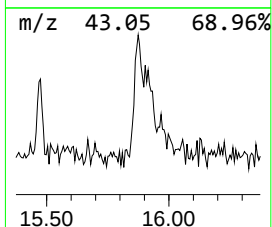
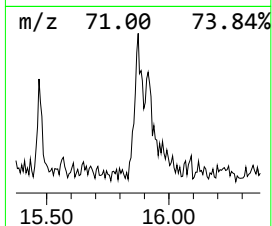
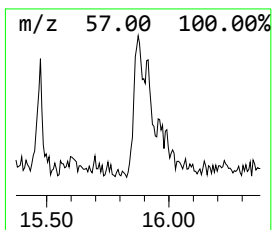
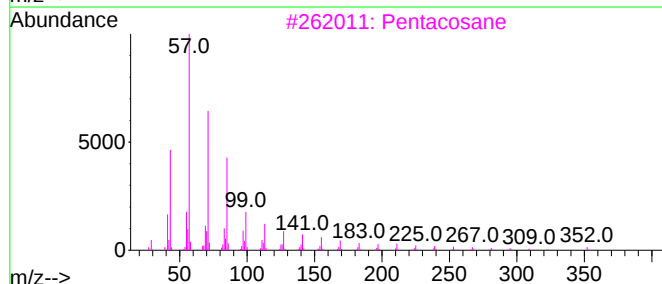
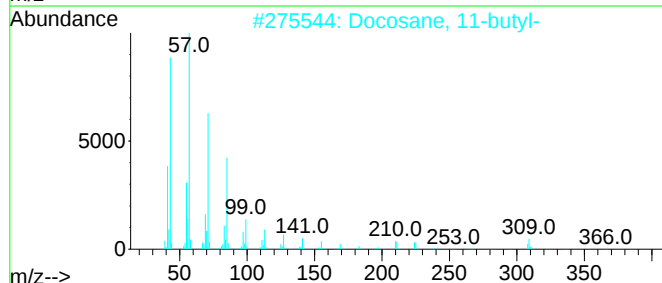
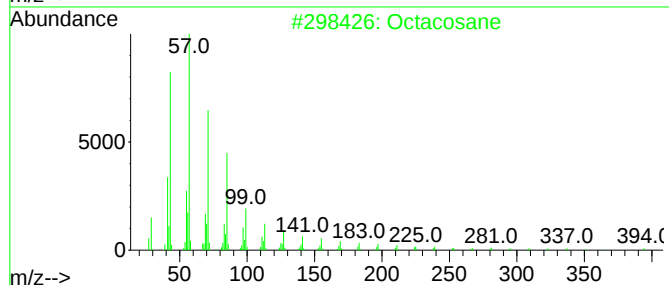
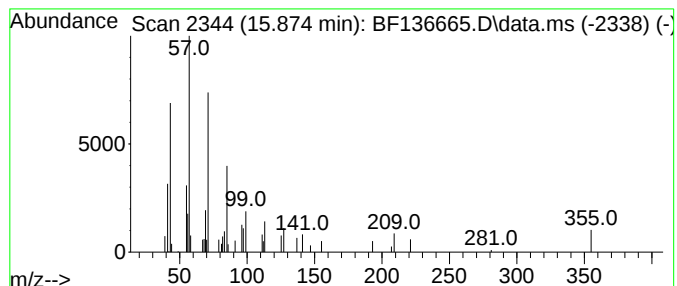
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Octacosane Concentration Rank 7

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.874 | 2.08 ng | 39067 | Perylene-d12     | 15.427 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------|-----|---------|-------------|------|
| 1    |    |   | Octacosane          | 394 | C28H58  | 000630-02-4 | 80   |
| 2    |    |   | Docosane, 11-butyl- | 366 | C26H54  | 013475-76-8 | 80   |
| 3    |    |   | Pentacosane         | 352 | C25H52  | 000629-99-2 | 80   |
| 4    |    |   | Hexacosane          | 366 | C26H54  | 000630-01-3 | 80   |
| 5    |    |   | Eicosane            | 282 | C20H42  | 000112-95-8 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122123\  
Data File : BF136665.D  
Acq On : 21 Dec 2023 12:11  
Operator : CG\JU  
Sample : 05585-02  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P3874-SP2

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122023.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| n-Hexadecanoic ... | 11.839 | 8.8     | ng    | 282434   | 4                     | 11.304 | 642189 | 20.0 |
| Octadecanoic acid  | 12.627 | 6.2     | ng    | 197513   | 4                     | 11.304 | 642189 | 20.0 |
| Pentacosane        | 13.268 | 7.0     | ng    | 145579   | 5                     | 13.957 | 416388 | 20.0 |
| Octacosane, 2-m... | 14.021 | 6.4     | ng    | 134167   | 5                     | 13.957 | 416388 | 20.0 |
| Heneicosane        | 14.598 | 4.7     | ng    | 98229    | 5                     | 13.957 | 416388 | 20.0 |
| Octadecane         | 15.198 | 3.3     | ng    | 61798    | 6                     | 15.427 | 375210 | 20.0 |
| Octacosane         | 15.874 | 2.1     | ng    | 39067    | 6                     | 15.427 | 375210 | 20.0 |