

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF080322\  
 Data File : BF129543.D  
 Acq On : 03 Aug 2022 16:36  
 Operator : CG\JU  
 Sample : PB146537BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB146537BL

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-BF072522.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129543.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         | 5.510       | 543           | 548         | 551          | rBV      | 5436700        | 5289980       | 78.21%          | 12.068%       |
| 2         | 6.516       | 713           | 719         | 722          | rBV      | 4983272        | 5331318       | 78.82%          | 12.163%       |
| 3         | 6.869       | 775           | 779         | 782          | rBV      | 1409627        | 1202318       | 17.78%          | 2.743%        |
| 4         | 7.434       | 869           | 875         | 878          | rBV      | 3231830        | 3663661       | 54.16%          | 8.358%        |
| 5         | 8.151       | 992           | 997         | 1000         | rBV      | 1885350        | 1647349       | 24.35%          | 3.758%        |
| 6         | 9.228       | 1174          | 1180        | 1183         | rBV      | 6734918        | 6659069       | 98.45%          | 15.192%       |
| 7         | 9.910       | 1290          | 1296        | 1299         | rBV      | 2093270        | 1885147       | 27.87%          | 4.301%        |
| 8         | 10.704      | 1424          | 1431        | 1434         | rBV      | 4297030        | 4027923       | 59.55%          | 9.189%        |
| 9         | 11.398      | 1545          | 1549        | 1553         | rBV      | 2202602        | 1855935       | 27.44%          | 4.234%        |
| 10        | 12.792      | 1783          | 1786        | 1789         | rVB      | 99709          | 80475         | 1.19%           | 0.184%        |
| 11        | 12.986      | 1814          | 1819        | 1823         | rBV      | 6357296        | 6764062       | 100.00%         | 15.431%       |
| 12        | 13.498      | 1902          | 1906        | 1910         | rBV      | 80776          | 72461         | 1.07%           | 0.165%        |
| 13        | 14.045      | 1994          | 1999        | 2002         | rBV      | 1631703        | 1523957       | 22.53%          | 3.477%        |
| 14        | 14.486      | 2071          | 2074        | 2078         | rBV      | 82609          | 82500         | 1.22%           | 0.188%        |
| 15        | 14.798      | 2123          | 2127        | 2131         | rVB      | 186385         | 184720        | 2.73%           | 0.421%        |
| 16        | 15.139      | 2180          | 2185        | 2190         | rBV      | 258474         | 298284        | 4.41%           | 0.680%        |
| 17        | 15.527      | 2245          | 2251        | 2257         | rBV2     | 1237373        | 1634866       | 24.17%          | 3.730%        |
| 18        | 15.963      | 2319          | 2325        | 2330         | rBV      | 307668         | 448758        | 6.63%           | 1.024%        |
| 19        | 16.468      | 2405          | 2411        | 2419         | rBV      | 246062         | 434721        | 6.43%           | 0.992%        |
| 20        | 17.068      | 2507          | 2513        | 2520         | rVB      | 145524         | 301201        | 4.45%           | 0.687%        |
| 21        | 17.780      | 2627          | 2634        | 2641         | rVB      | 115250         | 267764        | 3.96%           | 0.611%        |
| 22        | 18.621      | 2773          | 2777        | 2788         | rVB2     | 66311          | 176683        | 2.61%           | 0.403%        |

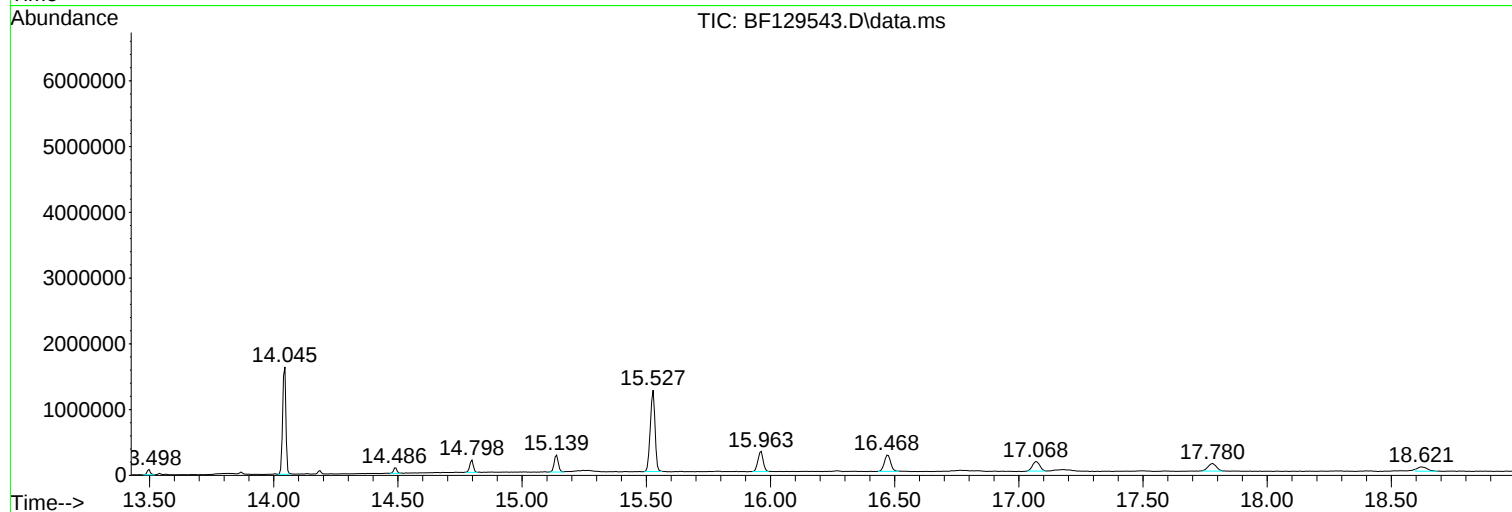
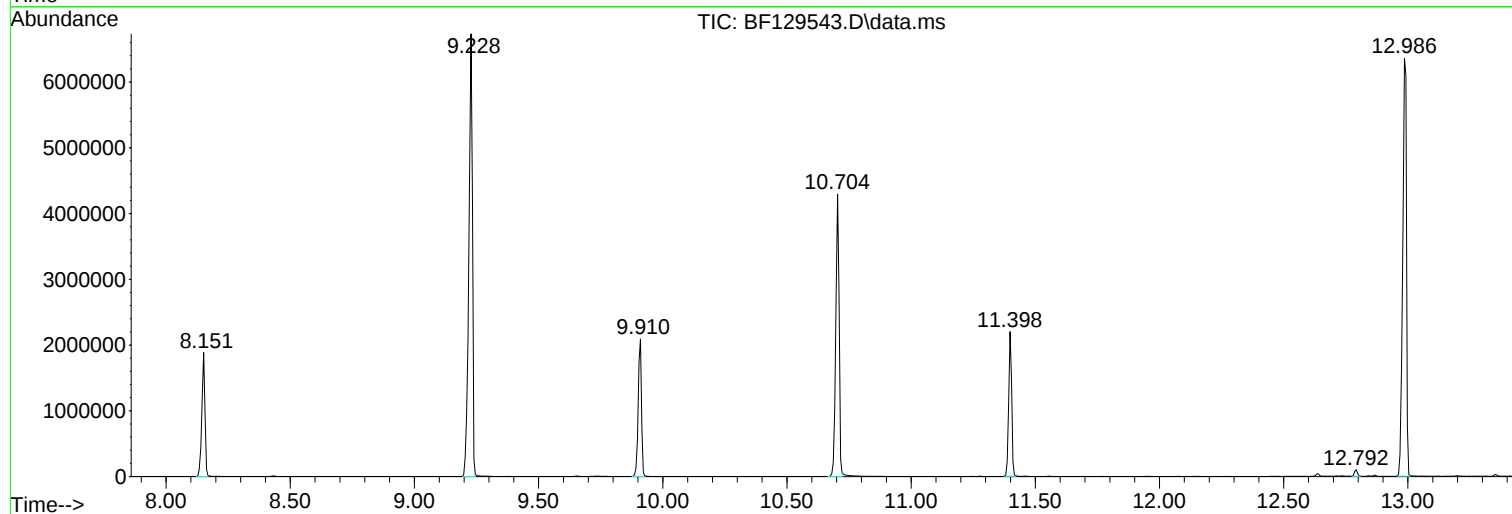
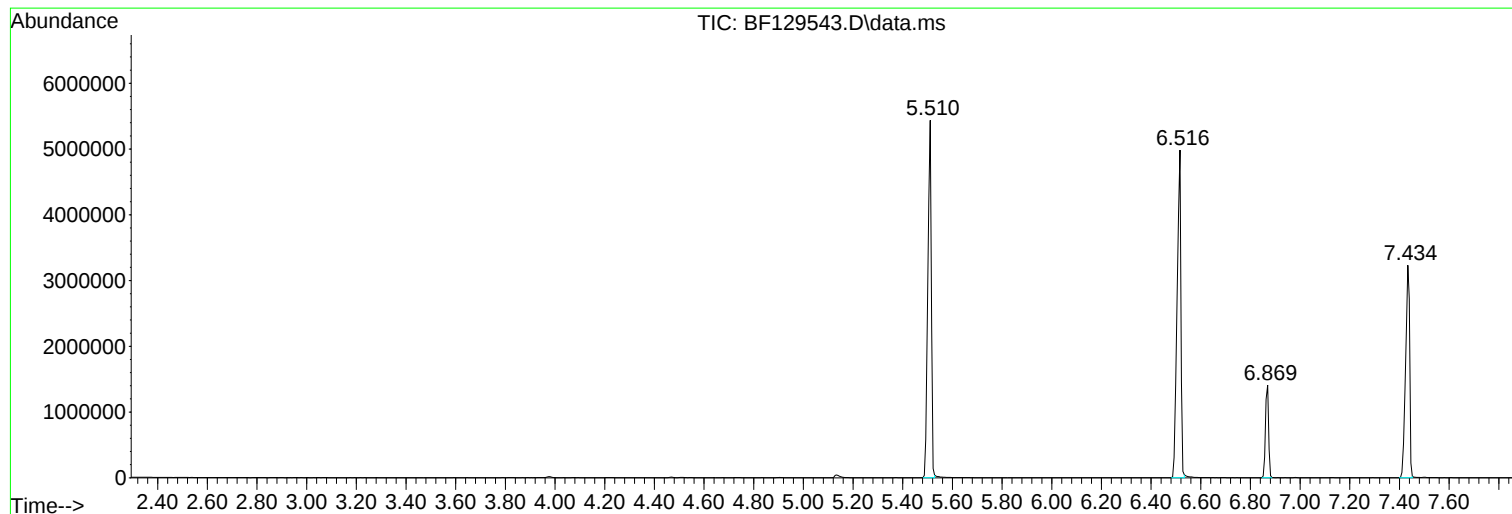
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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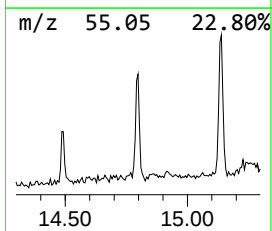
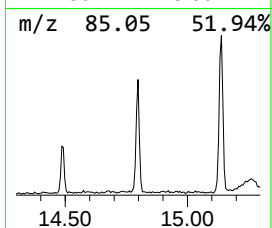
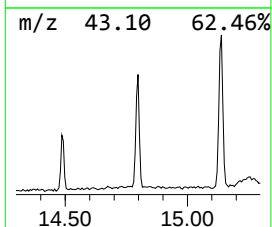
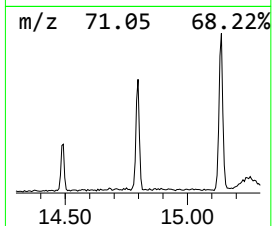
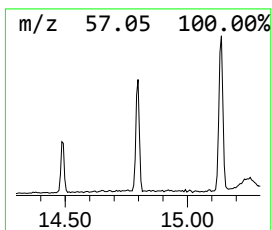
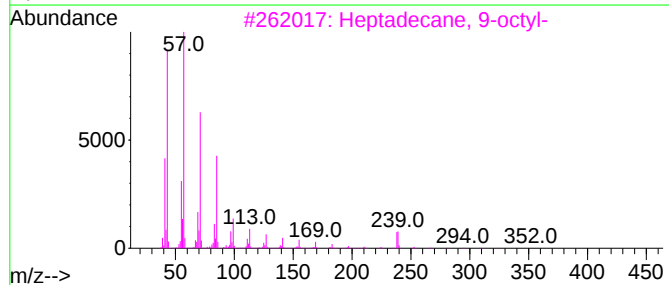
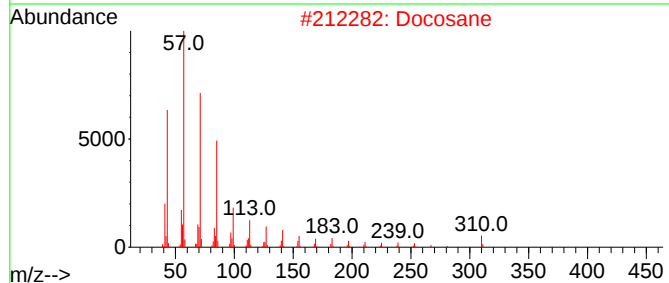
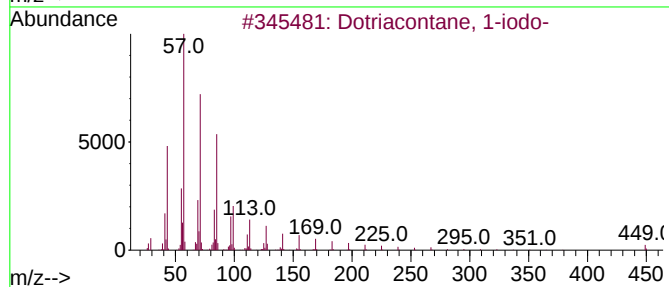
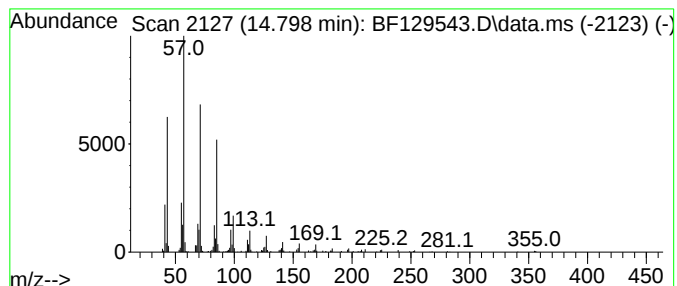
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 Dotriacontane, 1-iodo- Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.798 | 2.26 ng | 184720 | Perylene-d12     | 15.527 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------|-----|----------|--------------|------|
| 1    |    |   | Dotriacontane, 1-iodo-        | 576 | C32H65I  | 1000406-32-4 | 91   |
| 2    |    |   | Docosane                      | 310 | C22H46   | 000629-97-0  | 91   |
| 3    |    |   | Heptadecane, 9-octyl-         | 352 | C25H52   | 007225-64-1  | 91   |
| 4    |    |   | Pentadecane, 7-(bromomethyl)- | 304 | C16H33Br | 052997-43-0  | 91   |
| 5    |    |   | Heneicosane                   | 296 | C21H44   | 000629-94-7  | 90   |



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Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

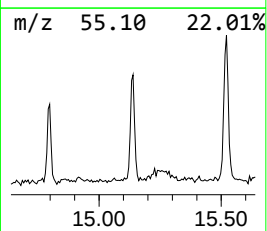
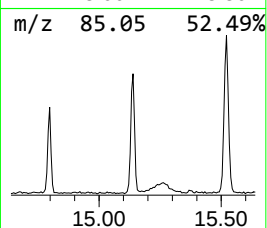
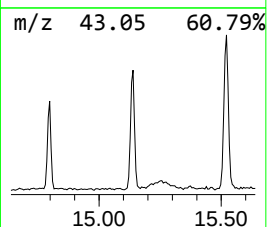
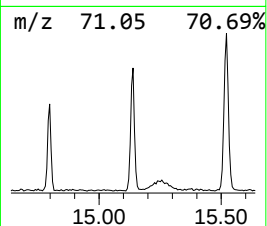
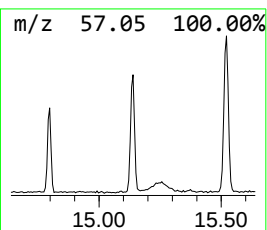
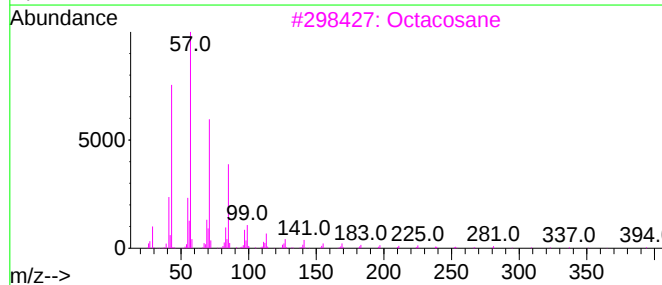
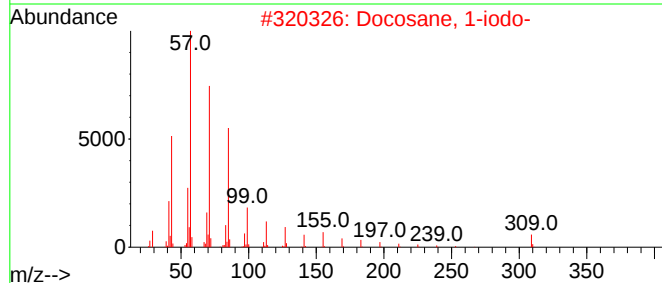
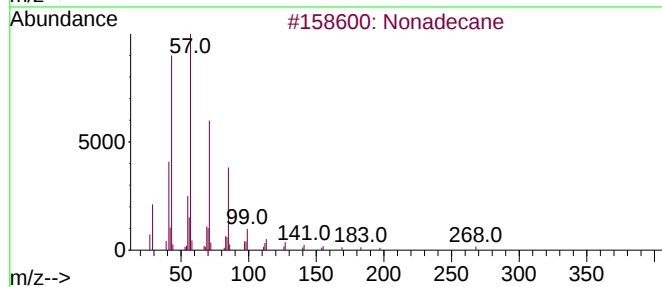
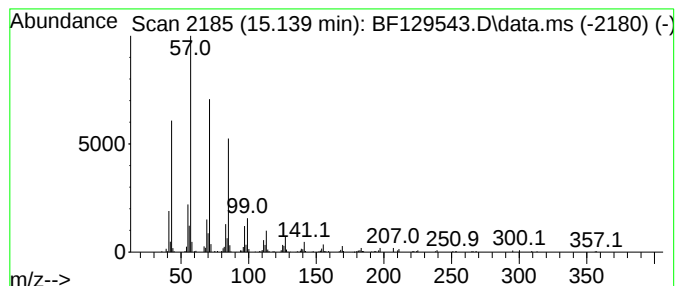
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Octacosane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.139 | 3.65 ng | 298284 | Perylene-d12     | 15.527 |

| Hit# | of 5 | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|------|------|-----------------------|-----|---------|--------------|------|
| 1    |      | Nonadecane            | 268 | C19H40  | 000629-92-5  | 93   |
| 2    |      | Docosane, 1-iodo-     | 436 | C22H45I | 1000406-31-9 | 91   |
| 3    |      | Octacosane            | 394 | C28H58  | 000630-02-4  | 91   |
| 4    |      | Tetracosane           | 338 | C24H50  | 000646-31-1  | 91   |
| 5    |      | Octacosane, 2-methyl- | 408 | C29H60  | 001560-98-1  | 91   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
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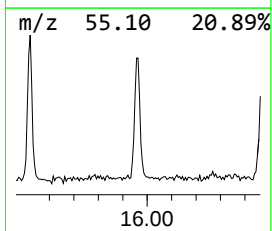
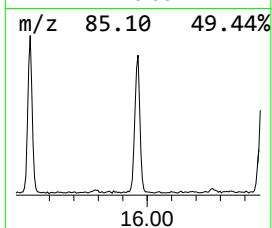
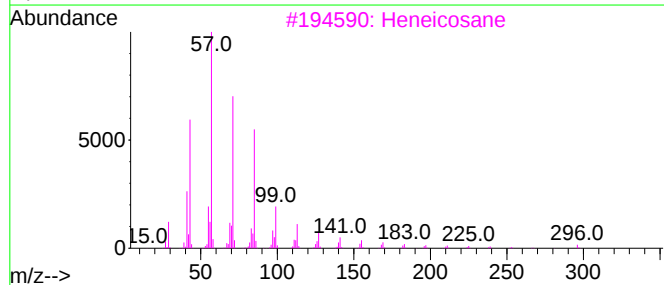
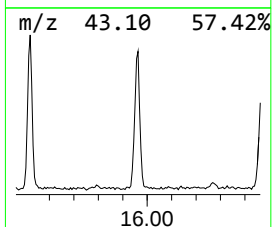
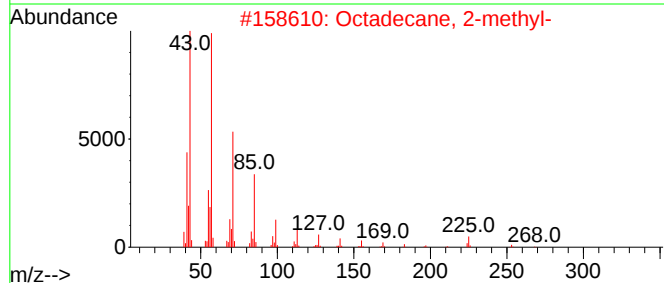
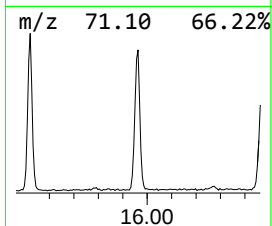
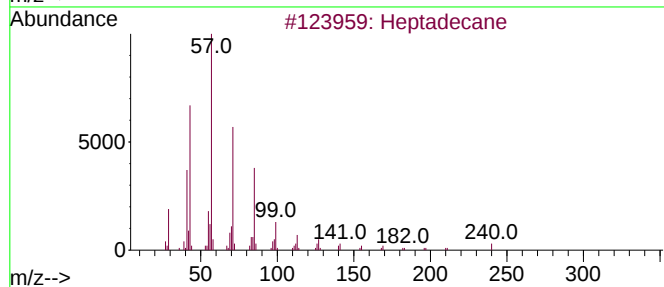
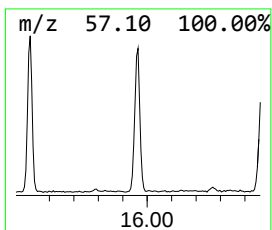
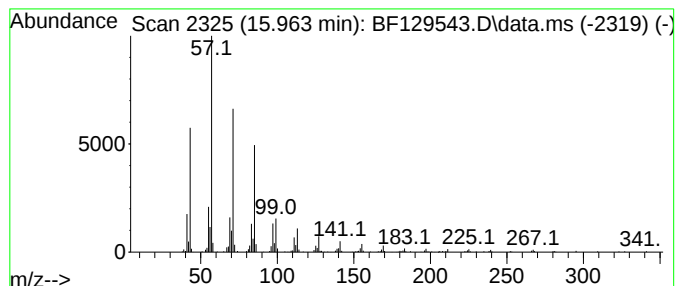
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Heptadecane Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.963 | 5.49 ng | 448758 | Perylene-d12     | 15.527 |

| Hit# | of | 5 | Tentative ID                     | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------|-----|---------|-------------|------|
| 1    |    |   | Heptadecane                      | 240 | C17H36  | 000629-78-7 | 94   |
| 2    |    |   | Octadecane, 2-methyl-            | 268 | C19H40  | 001560-88-9 | 94   |
| 3    |    |   | Heneicosane                      | 296 | C21H44  | 000629-94-7 | 91   |
| 4    |    |   | Octacosane                       | 394 | C28H58  | 000630-02-4 | 91   |
| 5    |    |   | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54  | 055282-11-6 | 91   |



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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

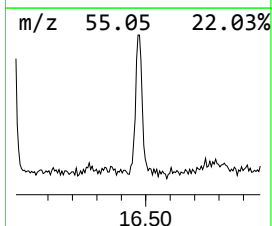
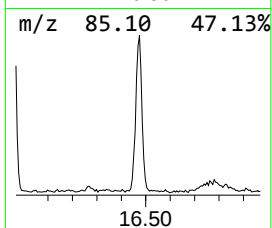
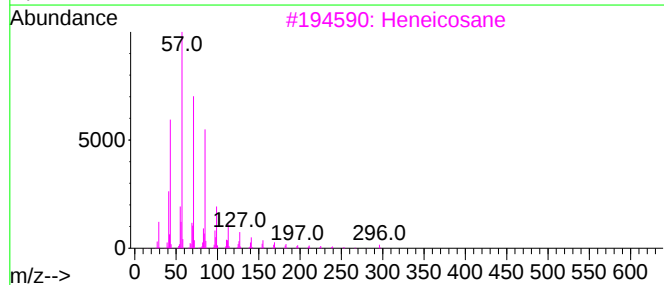
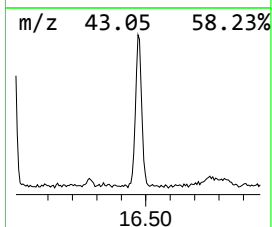
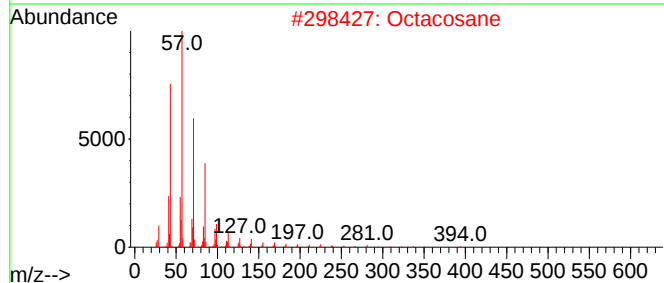
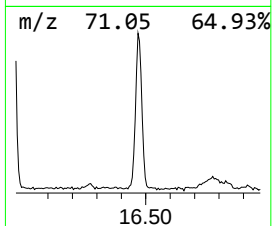
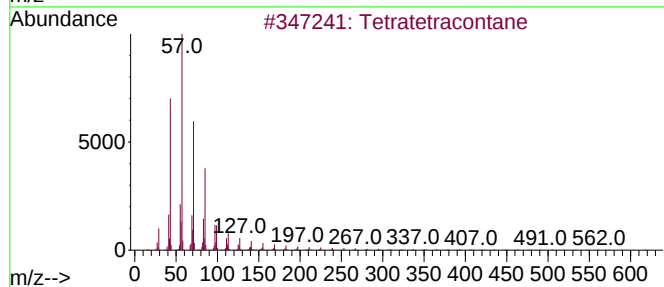
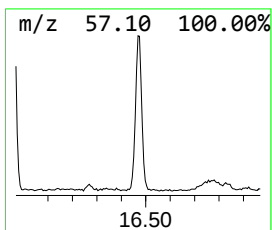
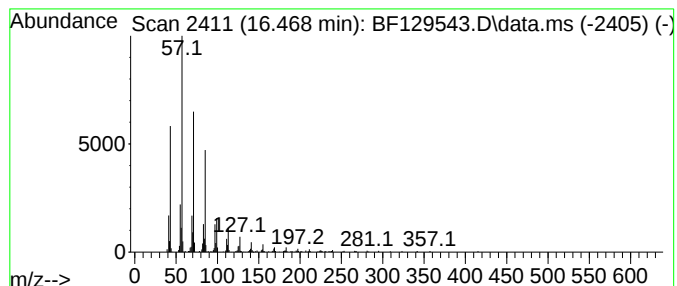
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tetratetracontane Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.468 | 5.32 ng | 434721 | Perylene-d12     | 15.527 |

| Hit# | of | 5 | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------|-----|---------|-------------|------|
| 1    |    |   | Tetratetracontane | 619 | C44H90  | 007098-22-8 | 91   |
| 2    |    |   | Octacosane        | 394 | C28H58  | 000630-02-4 | 91   |
| 3    |    |   | Heneicosane       | 296 | C21H44  | 000629-94-7 | 91   |
| 4    |    |   | Hexatriacontane   | 507 | C36H74  | 000630-06-8 | 91   |
| 5    |    |   | Tetracosane       | 338 | C24H50  | 000646-31-1 | 91   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

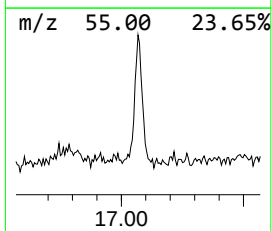
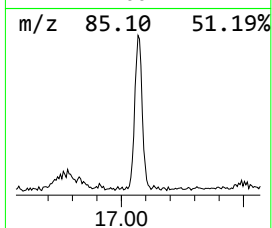
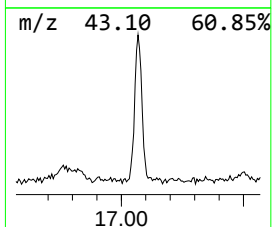
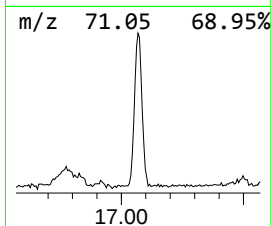
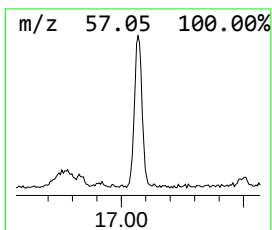
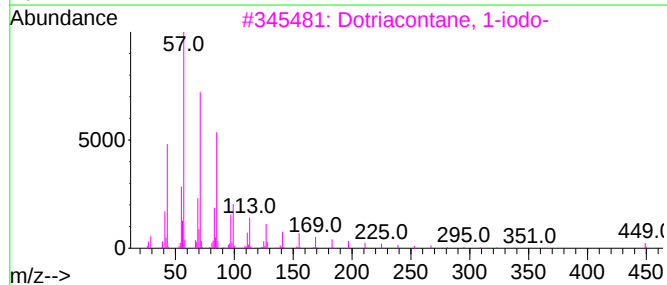
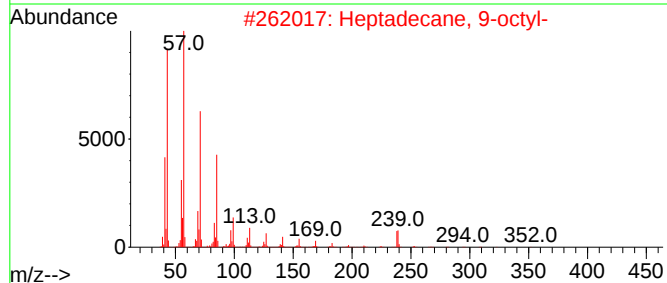
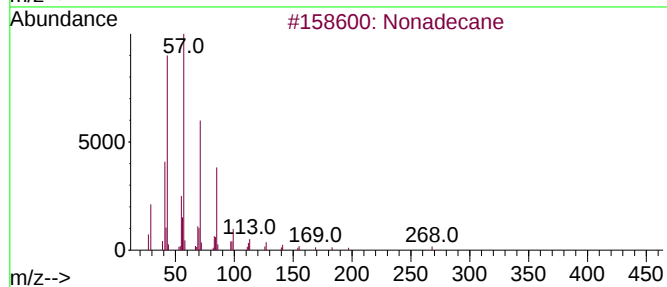
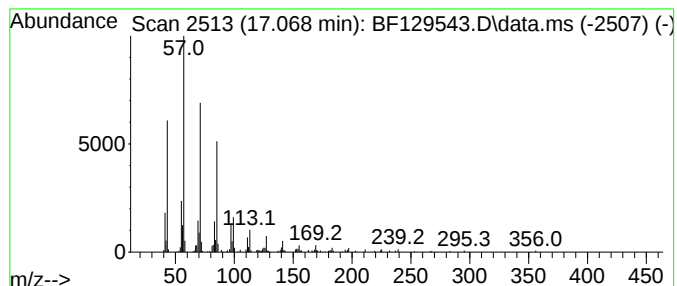
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Nonadecane Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.068 | 3.68 ng | 301201 | Perylene-d12     | 15.527 |

| Hit# | of | 5 | Tentative ID           | MW  | MolForm | CAS#         | Qual |
|------|----|---|------------------------|-----|---------|--------------|------|
| 1    |    |   | Nonadecane             | 268 | C19H40  | 000629-92-5  | 94   |
| 2    |    |   | Heptadecane, 9-octyl-  | 352 | C25H52  | 007225-64-1  | 91   |
| 3    |    |   | Dotriacontane, 1-iodo- | 576 | C32H65I | 1000406-32-4 | 91   |
| 4    |    |   | Tetracosane            | 338 | C24H50  | 000646-31-1  | 91   |
| 5    |    |   | Heneicosane            | 296 | C21H44  | 000629-94-7  | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF080322\  
Data File : BF129543.D  
Acq On : 03 Aug 2022 16:36  
Operator : CG\JU  
Sample : PB146537BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

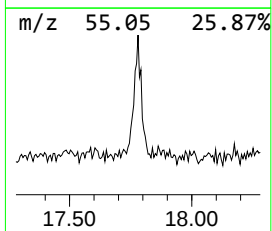
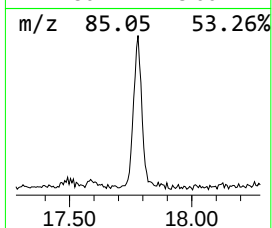
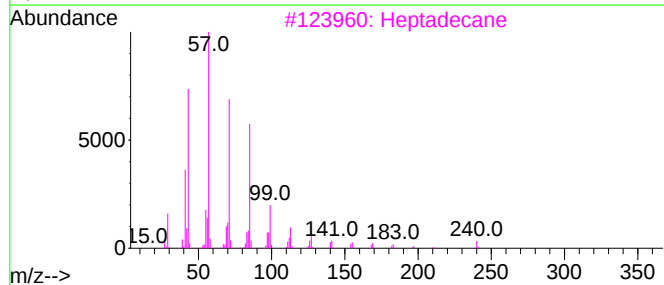
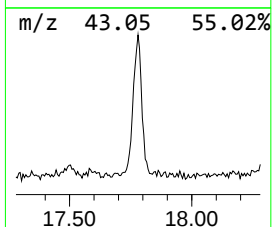
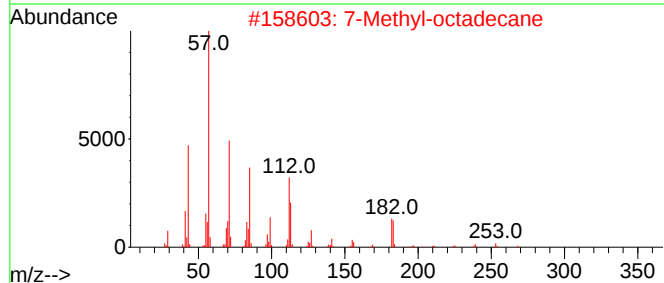
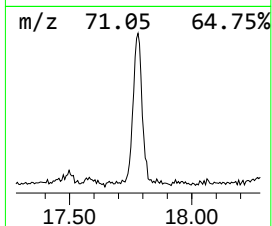
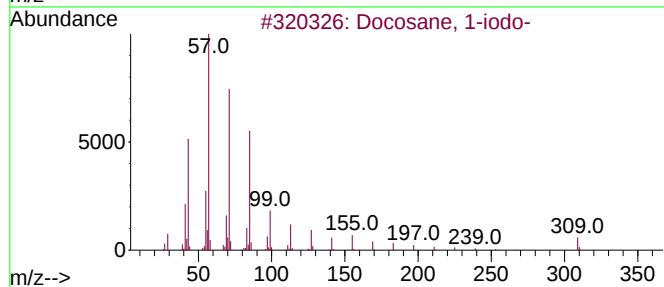
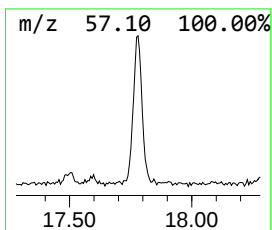
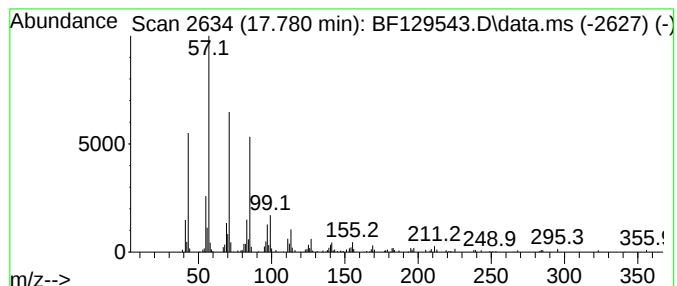
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Docosane, 1-iodo- Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.780 | 3.28 ng | 267764 | Perylene-d12     | 15.527 |

| Hit# | of 5 | Tentative ID         | MW  | MolForm | CAS#         | Qual |
|------|------|----------------------|-----|---------|--------------|------|
| 1    |      | Docosane, 1-iodo-    | 436 | C22H45I | 1000406-31-9 | 87   |
| 2    |      | 7-Methyl-octadecane  | 268 | C19H40  | 1000192-63-3 | 87   |
| 3    |      | Heptadecane          | 240 | C17H36  | 000629-78-7  | 86   |
| 4    |      | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1  | 83   |
| 5    |      | Octadecane           | 254 | C18H38  | 000593-45-3  | 83   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF080322\  
Data File : BF129543.D  
Acq On : 03 Aug 2022 16:36  
Operator : CG\JU  
Sample : PB146537BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

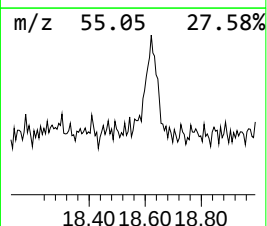
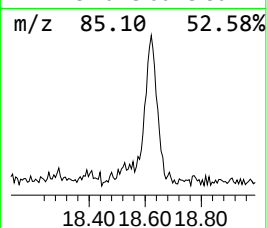
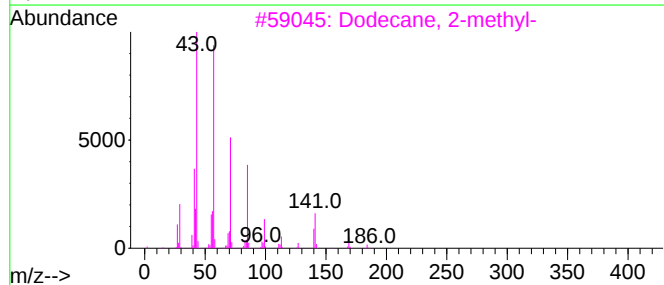
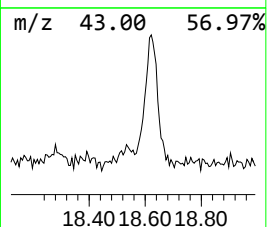
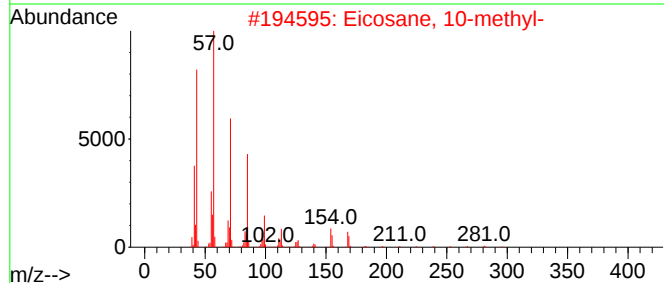
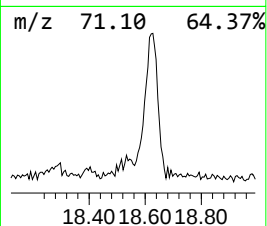
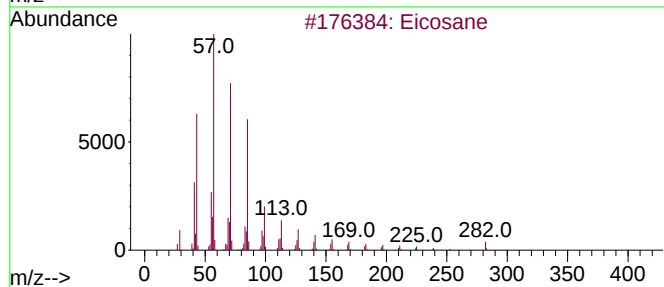
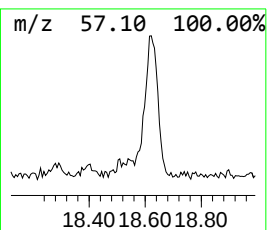
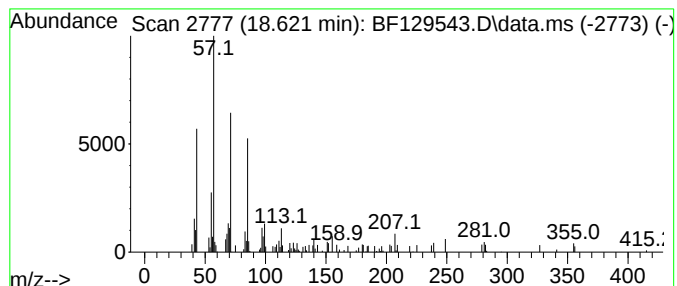
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Eicosane Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.621 | 2.16 ng | 176683 | Perylene-d12     | 15.527 |

| Hit# | of                   | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|------|----------------------|---|--------------|-----|---------|-------------|------|
| 1    | Eicosane             |   |              | 282 | C20H42  | 000112-95-8 | 81   |
| 2    | Eicosane, 10-methyl- |   |              | 296 | C21H44  | 054833-23-7 | 80   |
| 3    | Dodecane, 2-methyl-  |   |              | 184 | C13H28  | 001560-97-0 | 72   |
| 4    | Tridecane            |   |              | 184 | C13H28  | 000629-50-5 | 72   |
| 5    | Heneicosane          |   |              | 296 | C21H44  | 000629-94-7 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF080322\  
Data File : BF129543.D  
Acq On : 03 Aug 2022 16:36  
Operator : CG\JU  
Sample : PB146537BL  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB146537BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072522.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 |
| Dotriacontane, ... | 14.798 | 2.3     | ng    | 184720   | 6                     | 15.527 | 1634870 | 20.0 |
| Octacosane         | 15.139 | 3.6     | ng    | 298284   | 6                     | 15.527 | 1634870 | 20.0 |
| Heptadecane        | 15.963 | 5.5     | ng    | 448758   | 6                     | 15.527 | 1634870 | 20.0 |
| Tetratetracontane  | 16.468 | 5.3     | ng    | 434721   | 6                     | 15.527 | 1634870 | 20.0 |
| Nonadecane         | 17.068 | 3.7     | ng    | 301201   | 6                     | 15.527 | 1634870 | 20.0 |
| Docosane, 1-iodo-  | 17.780 | 3.3     | ng    | 267764   | 6                     | 15.527 | 1634870 | 20.0 |
| Eicosane           | 18.621 | 2.2     | ng    | 176683   | 6                     | 15.527 | 1634870 | 20.0 |