

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF041619\  
 Data File : BF113791.D  
 Acq On : 16 Apr 2019 14:00  
 Operator : JU/SJ  
 Sample : K2423-19  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP5-B

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-BF040319.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         | 4.881       | 472           | 475         | 489          | rBV      | 20448          | 38781         | 1.24%           | 0.141%        |
| 2         | 5.292       | 542           | 545         | 579          | rBV      | 2037579        | 2839774       | 90.99%          | 10.338%       |
| 3         | 6.334       | 718           | 722         | 738          | rBV      | 2401302        | 2967234       | 95.08%          | 10.802%       |
| 4         | 6.451       | 738           | 742         | 763          | rVB      | 2942570        | 3028117       | 97.03%          | 11.024%       |
| 5         | 6.669       | 776           | 779         | 793          | rVB      | 737718         | 708093        | 22.69%          | 2.578%        |
| 6         | 6.828       | 802           | 806         | 826          | rBV      | 2563767        | 2362676       | 75.71%          | 8.602%        |
| 7         | 7.239       | 872           | 876         | 906          | rBV      | 1721067        | 1924154       | 61.65%          | 7.005%        |
| 8         | 7.957       | 994           | 998         | 1016         | rBV      | 689922         | 883107        | 28.30%          | 3.215%        |
| 9         | 9.027       | 1176          | 1180        | 1192         | rBV      | 3391503        | 3120887       | 100.00%         | 11.362%       |
| 10        | 9.427       | 1245          | 1248        | 1261         | rBV      | 340998         | 376839        | 12.07%          | 1.372%        |
| 11        | 9.704       | 1291          | 1295        | 1312         | rBV      | 1013305        | 927912        | 29.73%          | 3.378%        |
| 12        | 10.498      | 1426          | 1430        | 1446         | rBV      | 1462249        | 1686956       | 54.05%          | 6.141%        |
| 13        | 11.186      | 1544          | 1547        | 1561         | rBV      | 759645         | 924188        | 29.61%          | 3.365%        |
| 14        | 11.727      | 1636          | 1639        | 1651         | rBV3     | 55351          | 98929         | 3.17%           | 0.360%        |
| 15        | 12.410      | 1751          | 1755        | 1760         | rBV      | 64276          | 72355         | 2.32%           | 0.263%        |
| 16        | 12.510      | 1769          | 1772        | 1778         | rBV2     | 42140          | 74167         | 2.38%           | 0.270%        |
| 17        | 12.633      | 1788          | 1793        | 1797         | rBV      | 59251          | 69965         | 2.24%           | 0.255%        |
| 18        | 12.768      | 1812          | 1816        | 1828         | rBV      | 2488028        | 2307203       | 73.93%          | 8.400%        |
| 19        | 13.339      | 1909          | 1913        | 1915         | rBV2     | 40482          | 37678         | 1.21%           | 0.137%        |
| 20        | 13.668      | 1965          | 1969        | 1972         | rVB      | 47277          | 43615         | 1.40%           | 0.159%        |
| 21        | 13.798      | 1987          | 1991        | 1993         | rBV      | 58006          | 57343         | 1.84%           | 0.209%        |
| 22        | 13.827      | 1993          | 1996        | 2005         | rVB      | 737441         | 801059        | 25.67%          | 2.916%        |
| 23        | 13.980      | 2019          | 2022        | 2027         | rVB      | 77681          | 70052         | 2.24%           | 0.255%        |
| 24        | 14.286      | 2070          | 2074        | 2078         | rVB      | 114112         | 104811        | 3.36%           | 0.382%        |
| 25        | 14.580      | 2120          | 2124        | 2128         | rBV      | 158539         | 154162        | 4.94%           | 0.561%        |
| 26        | 14.851      | 2166          | 2170        | 2172         | rBV      | 47368          | 59879         | 1.92%           | 0.218%        |
| 27        | 14.886      | 2172          | 2176        | 2183         | rVB2     | 189545         | 221433        | 7.10%           | 0.806%        |
| 28        | 15.127      | 2214          | 2217        | 2222         | rVB      | 28593          | 37122         | 1.19%           | 0.135%        |
| 29        | 15.239      | 2230          | 2236        | 2254         | rVB      | 735345         | 1082395       | 34.68%          | 3.941%        |
| 30        | 15.621      | 2296          | 2301        | 2307         | rVB      | 123998         | 172386        | 5.52%           | 0.628%        |
| 31        | 16.074      | 2373          | 2378        | 2392         | rBV2     | 70992          | 128182        | 4.11%           | 0.467%        |
| 32        | 16.598      | 2464          | 2467        | 2480         | rVB6     | 31093          | 86703         | 2.78%           | 0.316%        |

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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-BF040319.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

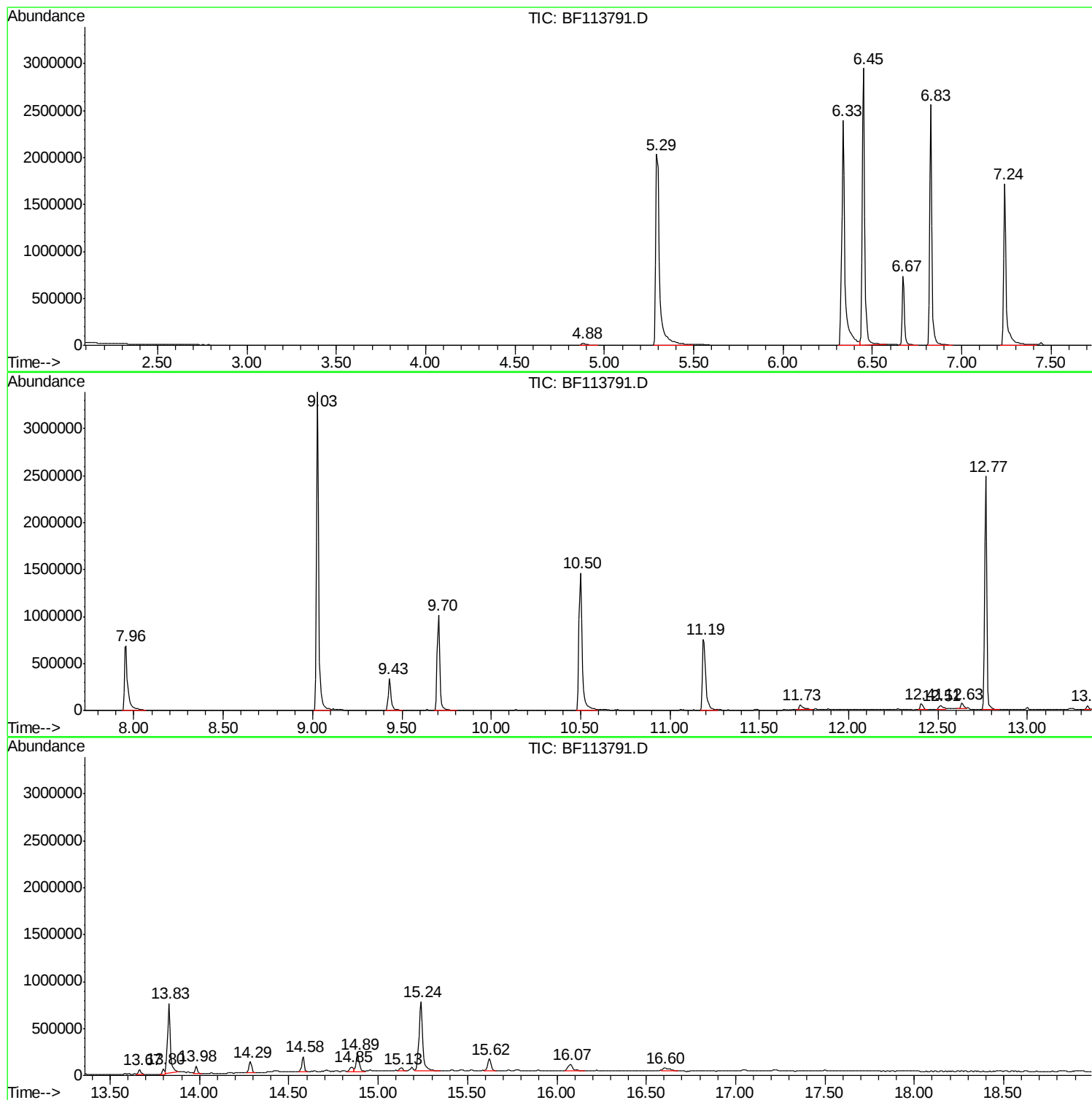
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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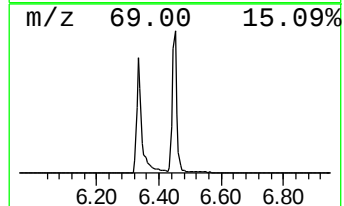
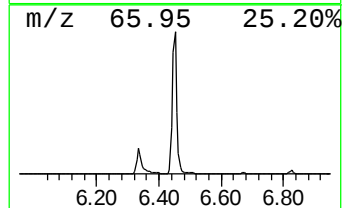
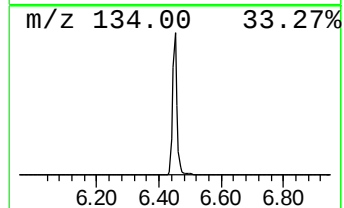
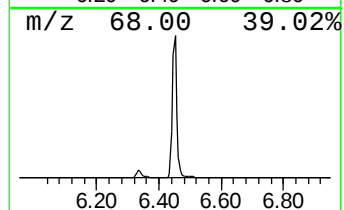
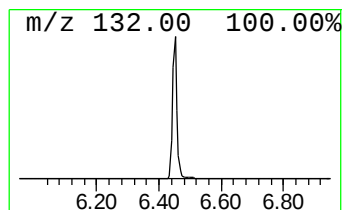
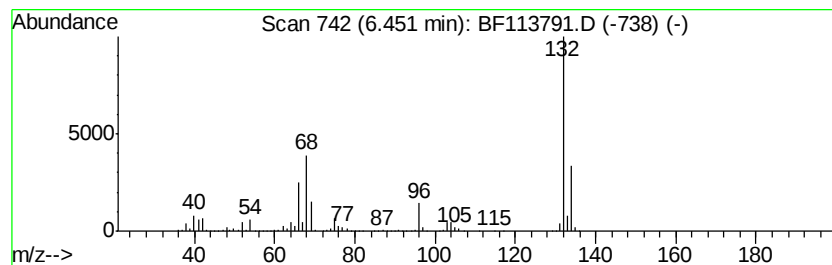
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.45 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.45 | 85.53 ng | 3028120 | 1,4-Dichlorobenzene-d4 | 6.67 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 16   |
| 3    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 5    |    | Xenon                            | 132 | Xe        | 007440-63-3  | 9    |



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Instrument :  
BNA\_F  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

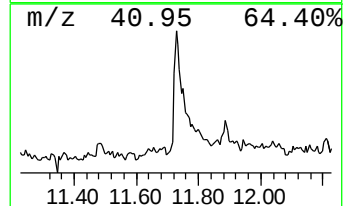
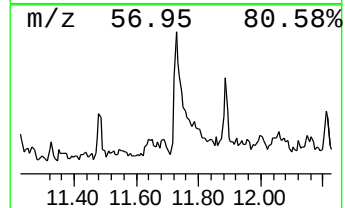
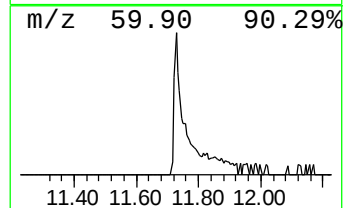
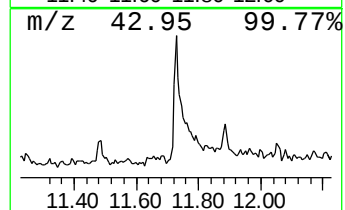
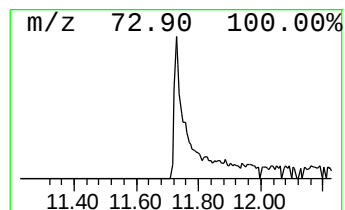
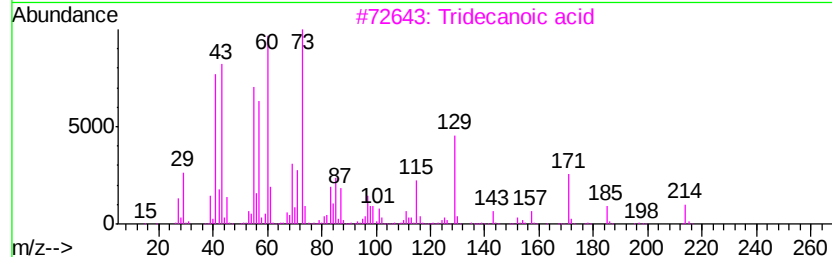
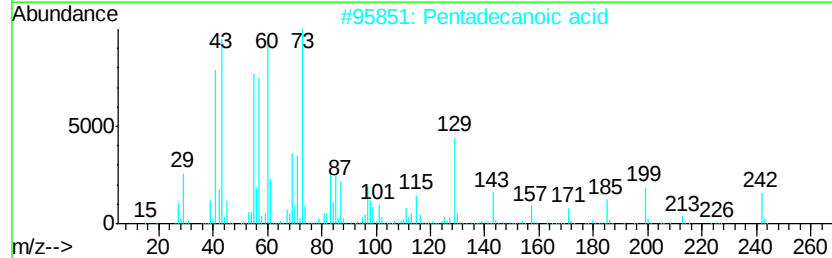
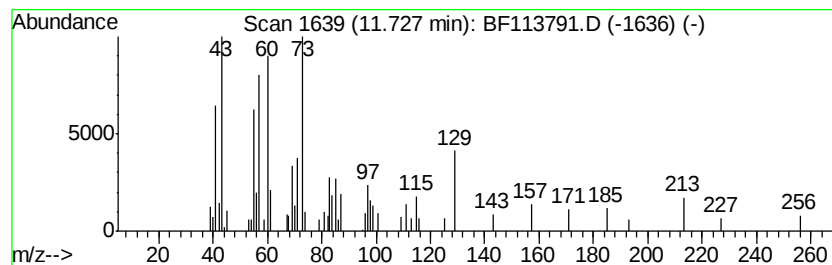
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 11.73 | 2.14 ng | 98929 | Phenanthrene-d10 | 11.19 |

| Hit# of | 5 | Tentative ID                   | MW  | MolForm    | CAS#        | Qual |
|---------|---|--------------------------------|-----|------------|-------------|------|
| 1       |   | n-Hexadecanoic acid            | 256 | C16H32O2   | 000057-10-3 | 98   |
| 2       |   | Pentadecanoic acid             | 242 | C15H30O2   | 001002-84-2 | 87   |
| 3       |   | Tridecanoic acid               | 214 | C13H26O2   | 000638-53-9 | 80   |
| 4       |   | Tetradecanoic acid             | 228 | C14H28O2   | 000544-63-8 | 78   |
| 5       |   | Decanoic acid, silver(1+) salt | 278 | C10H19AgO2 | 013126-67-5 | 72   |



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Instrument :  
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TP5-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

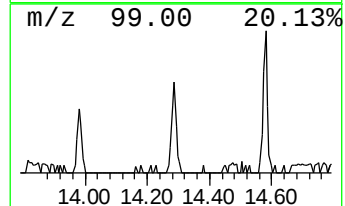
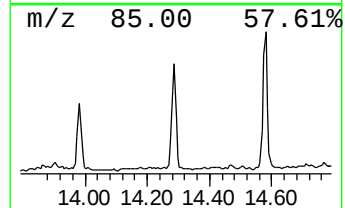
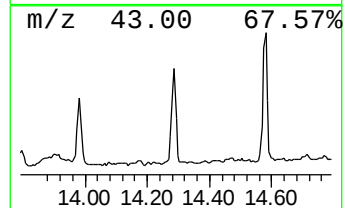
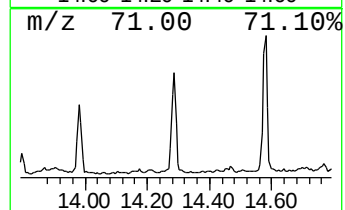
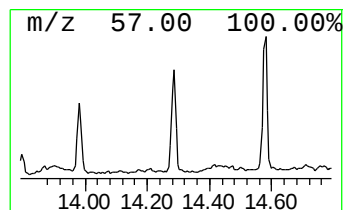
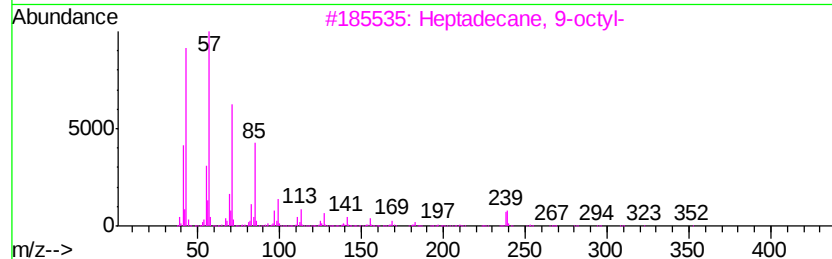
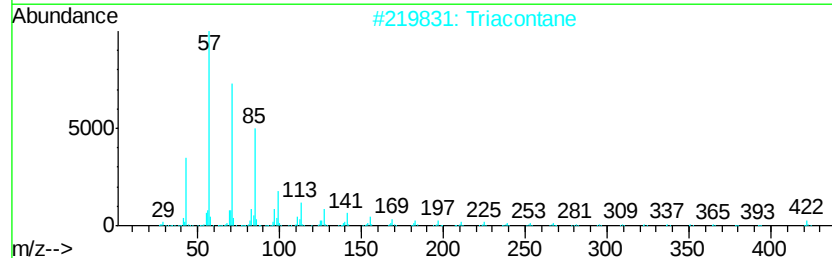
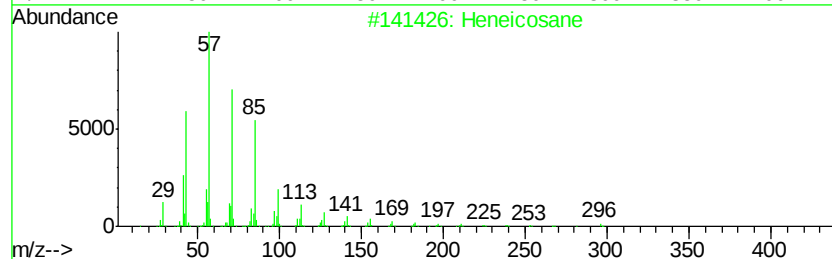
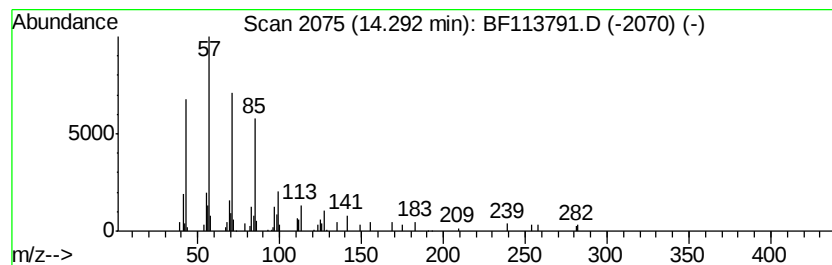
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Heneicosane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.29 | 2.62 ng | 104811 | Chrysene-d12     | 13.83 |

| Hit# of | 5                     | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-----------------------|--------------|-----|---------|-------------|------|
| 1       | Heneicosane           |              | 296 | C21H44  | 000629-94-7 | 91   |
| 2       | Triacontane           |              | 422 | C30H62  | 000638-68-6 | 91   |
| 3       | Heptadecane, 9-octyl- |              | 352 | C25H52  | 007225-64-1 | 91   |
| 4       | Docosane              |              | 310 | C22H46  | 000629-97-0 | 91   |
| 5       | Heptadecane           |              | 240 | C17H36  | 000629-78-7 | 87   |



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Instrument :  
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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

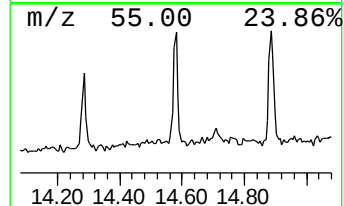
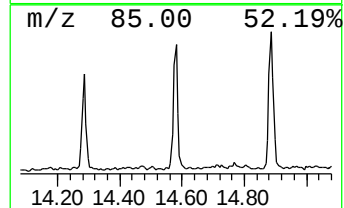
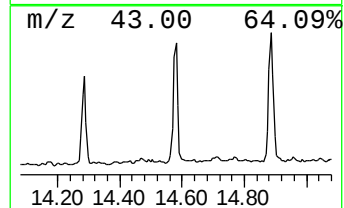
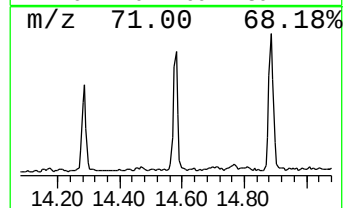
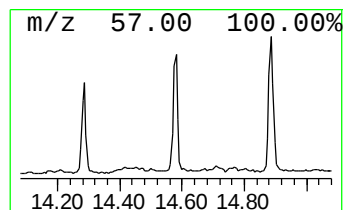
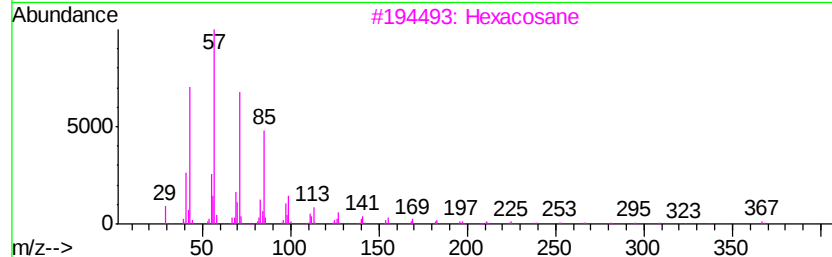
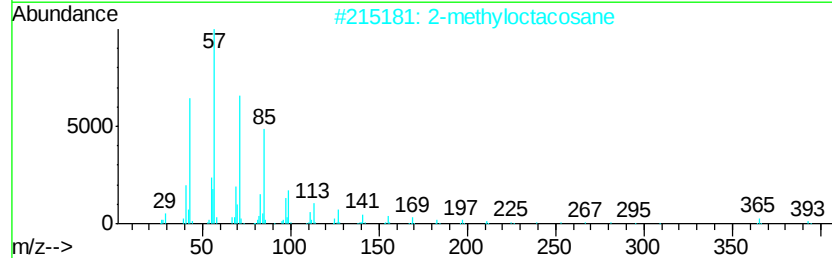
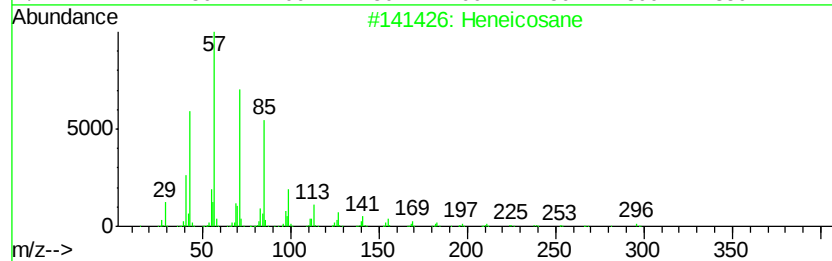
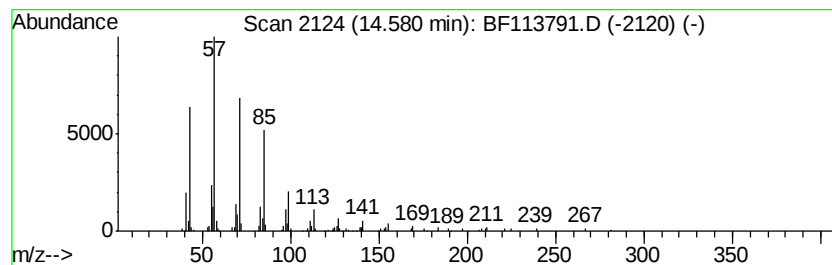
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 2-methyloctacosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.58 | 2.85 ng | 154162 | Perylene-d12     | 15.24 |

| Hit# of | 5 | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|---------|---|-----------------------|-----|---------|--------------|------|
| 1       |   | Heneicosane           | 296 | C21H44  | 000629-94-7  | 91   |
| 2       |   | 2-methyloctacosane    | 408 | C29H60  | 1000376-72-8 | 91   |
| 3       |   | Hexacosane            | 366 | C26H54  | 000630-01-3  | 87   |
| 4       |   | Hexadecane, 1-iodo-   | 352 | C16H33I | 000544-77-4  | 87   |
| 5       |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1  | 86   |



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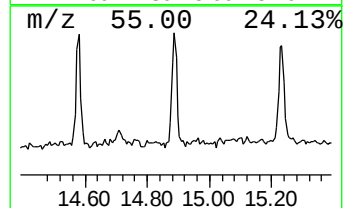
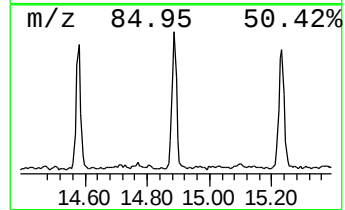
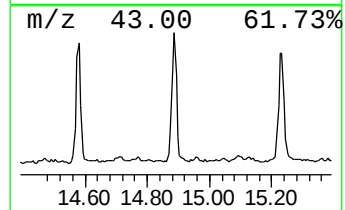
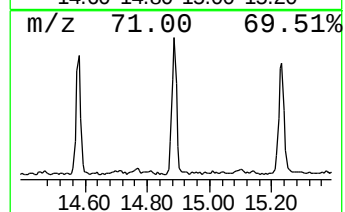
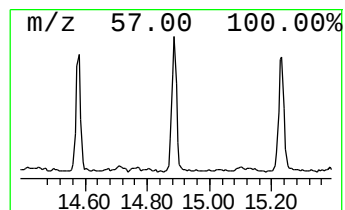
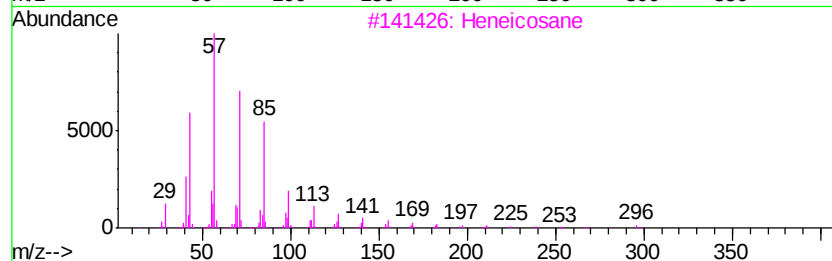
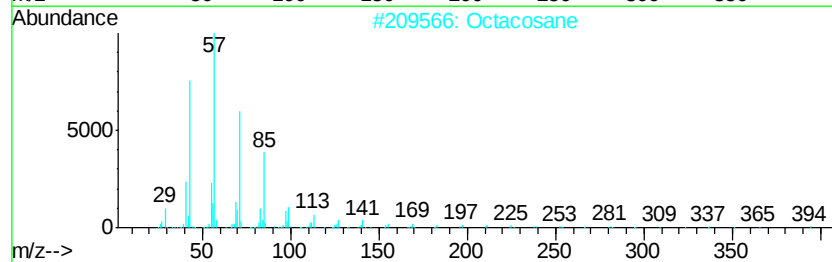
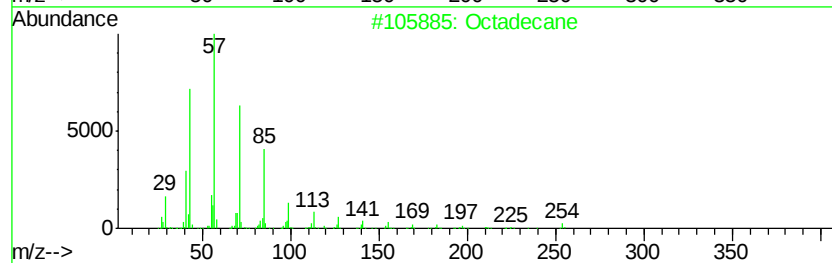
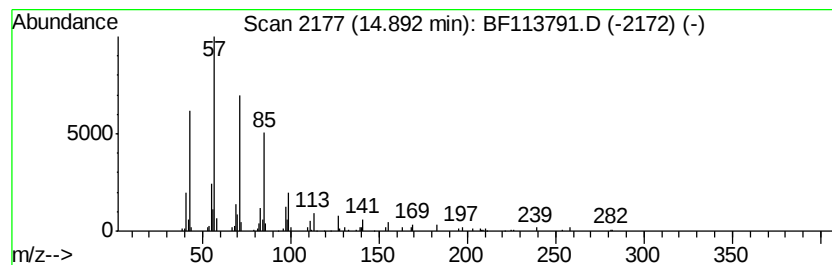
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 6 Octadecane Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.89 | 4.09 ng | 221433 | Perylene-d12     | 15.24 |

| Hit# of | 5           | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------|--------------|-----|---------|-------------|------|
| 1       | Octadecane  |              | 254 | C18H38  | 000593-45-3 | 95   |
| 2       | Octacosane  |              | 394 | C28H58  | 000630-02-4 | 91   |
| 3       | Heneicosane |              | 296 | C21H44  | 000629-94-7 | 91   |
| 4       | Triacotane  |              | 422 | C30H62  | 000638-68-6 | 91   |
| 5       | Tetracosane |              | 338 | C24H50  | 000646-31-1 | 87   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF041619\  
Data File : BF113791.D  
Acq On : 16 Apr 2019 14:00  
Operator : JU/SJ  
Sample : K2423-19  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP5-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

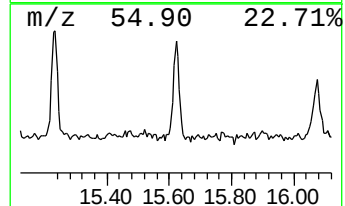
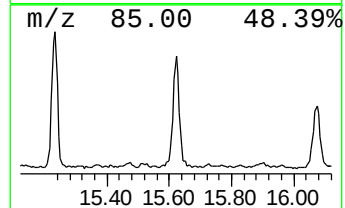
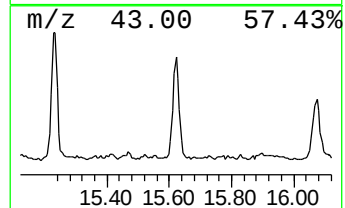
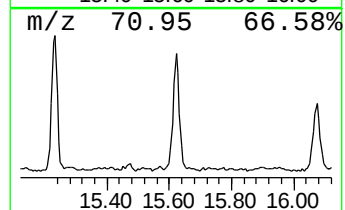
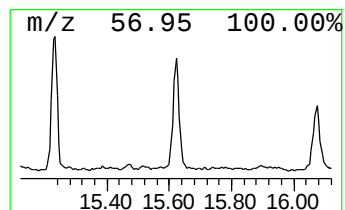
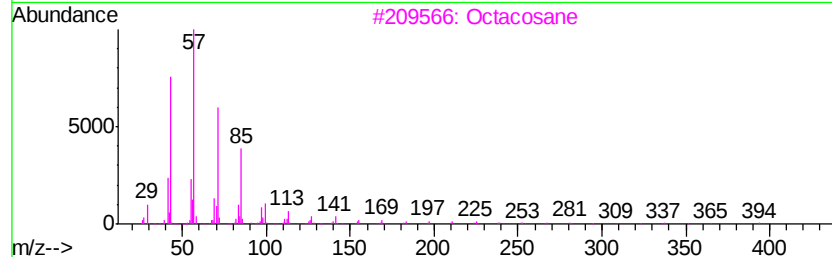
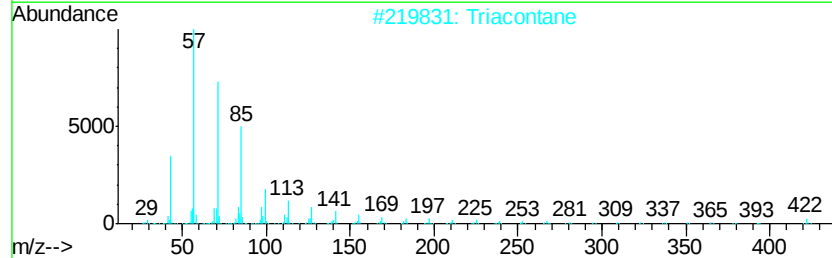
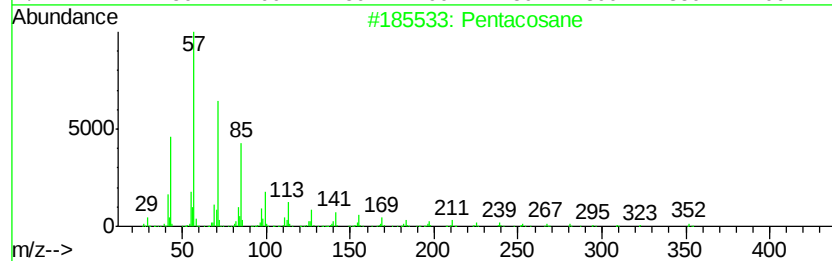
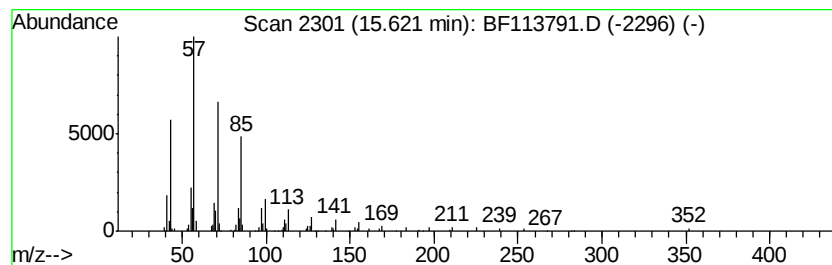
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Pentacosane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.62 | 3.19 ng | 172386 | Perylene-d12     | 15.24 |

| Hit# of | 5           | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------|--------------|-----|---------|-------------|------|
| 1       | Pentacosane |              | 352 | C25H52  | 000629-99-2 | 95   |
| 2       | triacontane |              | 422 | C30H62  | 000638-68-6 | 91   |
| 3       | Octacosane  |              | 394 | C28H58  | 000630-02-4 | 91   |
| 4       | Heneicosane |              | 296 | C21H44  | 000629-94-7 | 91   |
| 5       | Hexacosane  |              | 366 | C26H54  | 000630-01-3 | 91   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF041619\  
Data File : BF113791.D  
Acq On : 16 Apr 2019 14:00  
Operator : JU/SJ  
Sample : K2423-19  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP5-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

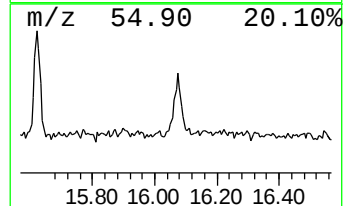
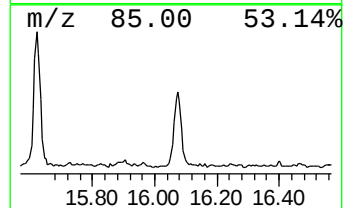
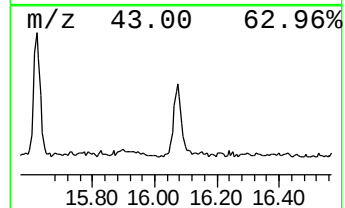
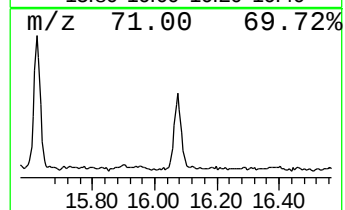
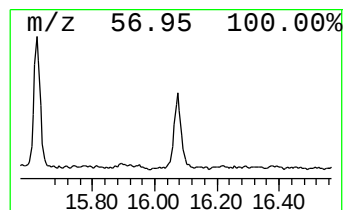
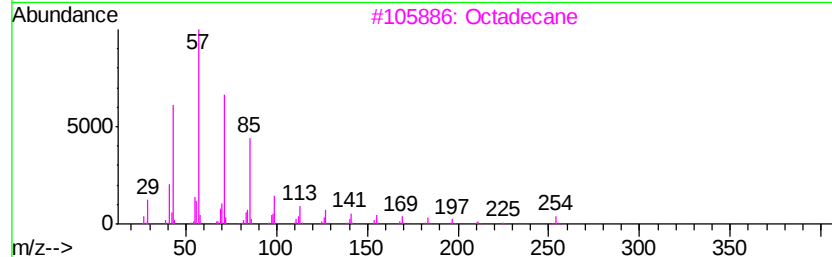
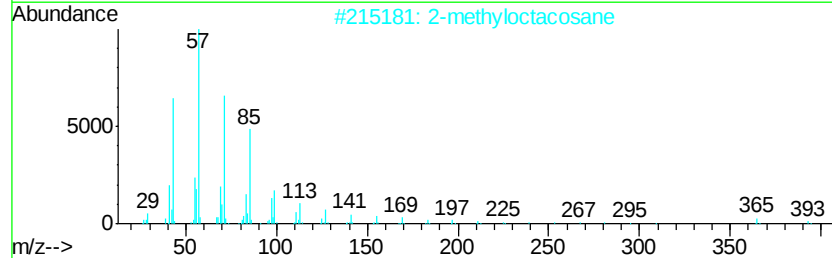
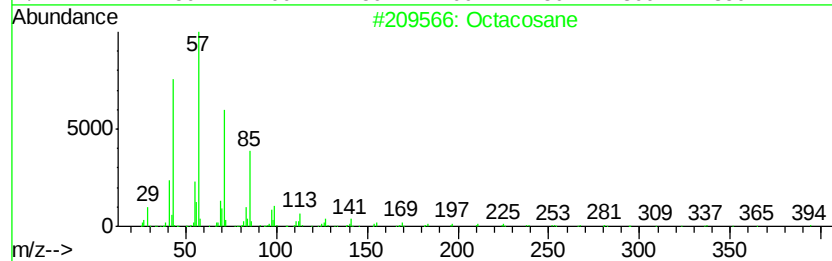
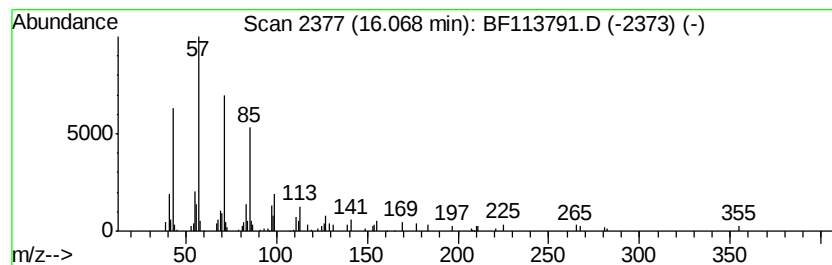
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Octacosane Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.07 | 2.37 ng | 128182 | Perylene-d12     | 15.24 |

| Hit# | of | Tentative ID       | MW  | MolForm | CAS#         | Qual |
|------|----|--------------------|-----|---------|--------------|------|
| 1    | 5  | Octacosane         | 394 | C28H58  | 000630-02-4  | 90   |
| 2    |    | 2-methyloctacosane | 408 | C29H60  | 1000376-72-8 | 90   |
| 3    |    | Octadecane         | 254 | C18H38  | 000593-45-3  | 87   |
| 4    |    | Heneicosane        | 296 | C21H44  | 000629-94-7  | 87   |
| 5    |    | triacontane        | 422 | C30H62  | 000638-68-6  | 87   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF041619\  
Data File : BF113791.D  
Acq On : 16 Apr 2019 14:00  
Operator : JU/SJ  
Sample : K2423-19  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TP5-B

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF040319.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 |
| unknown6.45         | 6.45  | 85.5    | ng    | 3028120  | 1                     | 6.67  | 708093  | 20.0 |
| n-Hexadecanoic acid | 11.73 | 2.1     | ng    | 98929    | 4                     | 11.19 | 924188  | 20.0 |
| Heneicosane         | 14.29 | 2.6     | ng    | 104811   | 5                     | 13.83 | 801059  | 20.0 |
| 2-methyloctacosane  | 14.58 | 2.9     | ng    | 154162   | 6                     | 15.24 | 1082400 | 20.0 |
| Octadecane          | 14.89 | 4.1     | ng    | 221433   | 6                     | 15.24 | 1082400 | 20.0 |
| Pentacosane         | 15.62 | 3.2     | ng    | 172386   | 6                     | 15.24 | 1082400 | 20.0 |
| Octacosane          | 16.07 | 2.4     | ng    | 128182   | 6                     | 15.24 | 1082400 | 20.0 |