

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF051019\  
 Data File : BF114145.D  
 Acq On : 11 May 2019 2:18  
 Operator : JU/SJ  
 Sample : K2750-03 10X  
 Misc :  
 ALS Vial : 23 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 72-11995

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-BF051019.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.475       | 573           | 576         | 587          | rBV      | 474704         | 491804        | 22.80%          | 2.861%        |
| 2         | 6.487       | 744           | 748         | 758          | rBV      | 542962         | 555324        | 25.74%          | 3.230%        |
| 3         | 6.622       | 768           | 771         | 779          | rBV      | 558950         | 523813        | 24.28%          | 3.047%        |
| 4         | 6.857       | 807           | 811         | 814          | rBV      | 1867963        | 1688723       | 78.28%          | 9.824%        |
| 5         | 7.010       | 834           | 837         | 843          | rVB      | 496265         | 400345        | 18.56%          | 2.329%        |
| 6         | 7.410       | 901           | 905         | 917          | rVB      | 290669         | 260058        | 12.06%          | 1.513%        |
| 7         | 8.133       | 1025          | 1028        | 1032         | rBV      | 2415676        | 1972165       | 91.42%          | 11.472%       |
| 8         | 8.563       | 1098          | 1101        | 1107         | rVB3     | 25865          | 29649         | 1.37%           | 0.172%        |
| 9         | 9.204       | 1207          | 1210        | 1221         | rBV      | 616824         | 524377        | 24.31%          | 3.050%        |
| 10        | 9.792       | 1304          | 1310        | 1317         | rVB3     | 30153          | 58705         | 2.72%           | 0.341%        |
| 11        | 9.886       | 1323          | 1326        | 1330         | rBV      | 2100859        | 1900051       | 88.08%          | 11.053%       |
| 12        | 10.092      | 1357          | 1361        | 1368         | rBV5     | 25710          | 36274         | 1.68%           | 0.211%        |
| 13        | 10.675      | 1456          | 1460        | 1470         | rBV      | 289553         | 259118        | 12.01%          | 1.507%        |
| 14        | 11.327      | 1567          | 1571        | 1575         | rBV      | 63844          | 58386         | 2.71%           | 0.340%        |
| 15        | 11.374      | 1575          | 1579        | 1582         | rBV      | 2360244        | 2157204       | 100.00%         | 12.549%       |
| 16        | 11.898      | 1665          | 1668        | 1671         | rBV3     | 30313          | 36783         | 1.71%           | 0.214%        |
| 17        | 11.927      | 1671          | 1673        | 1676         | rVB      | 91937          | 75353         | 3.49%           | 0.438%        |
| 18        | 12.457      | 1761          | 1763        | 1769         | rVB2     | 30150          | 33754         | 1.56%           | 0.196%        |
| 19        | 12.710      | 1804          | 1806        | 1810         | rVB4     | 29487          | 26262         | 1.22%           | 0.153%        |
| 20        | 12.833      | 1824          | 1827        | 1828         | rBV      | 44278          | 38357         | 1.78%           | 0.223%        |
| 21        | 12.851      | 1828          | 1830        | 1831         | rBV2     | 34165          | 26729         | 1.24%           | 0.155%        |
| 22        | 12.951      | 1843          | 1847        | 1852         | rBV      | 747532         | 622944        | 28.88%          | 3.624%        |
| 23        | 13.186      | 1884          | 1887        | 1890         | rBV      | 82641          | 80429         | 3.73%           | 0.468%        |
| 24        | 13.527      | 1943          | 1945        | 1947         | rVB      | 108624         | 85652         | 3.97%           | 0.498%        |
| 25        | 13.639      | 1961          | 1964        | 1967         | rVB2     | 87376          | 73986         | 3.43%           | 0.430%        |
| 26        | 13.857      | 1998          | 2001        | 2007         | rBV      | 202392         | 206341        | 9.57%           | 1.200%        |
| 27        | 14.010      | 2023          | 2027        | 2030         | rVB      | 2038366        | 1719571       | 79.71%          | 10.003%       |
| 28        | 14.174      | 2052          | 2055        | 2057         | rBV      | 217552         | 191070        | 8.86%           | 1.111%        |
| 29        | 14.480      | 2104          | 2107        | 2110         | rBV      | 409767         | 349855        | 16.22%          | 2.035%        |
| 30        | 14.786      | 2156          | 2159        | 2163         | rVB      | 329472         | 294229        | 13.64%          | 1.712%        |
| 31        | 15.121      | 2213          | 2216        | 2220         | rBV      | 298604         | 337957        | 15.67%          | 1.966%        |
| 32        | 15.480      | 2273          | 2277        | 2287         | rVB      | 1137613        | 1637380       | 75.90%          | 9.525%        |
| 33        | 15.745      | 2318          | 2322        | 2330         | rVB      | 324159         | 437987        | 20.30%          | 2.548%        |

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ALS Vial : 23 Sample Multiplier: 1

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ClientSampleId :  
72-11995

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-BF051019.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

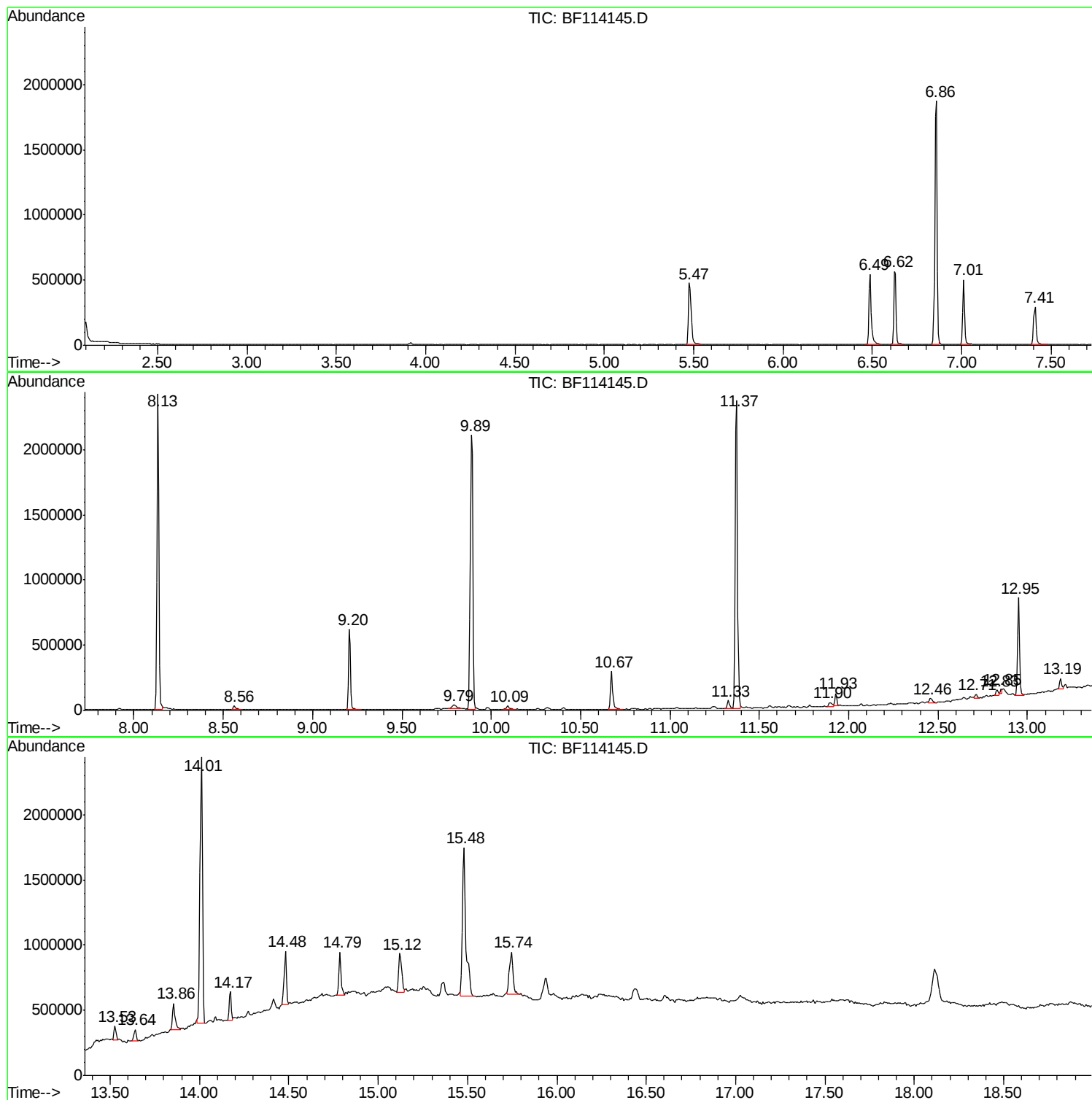
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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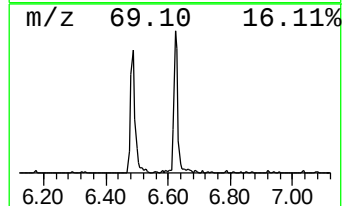
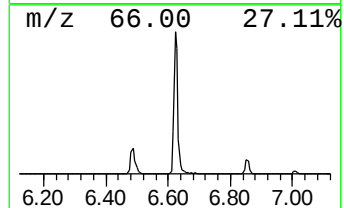
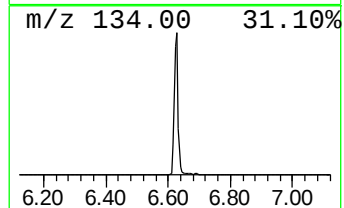
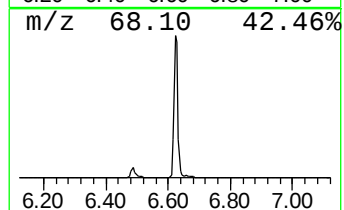
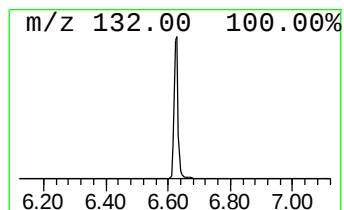
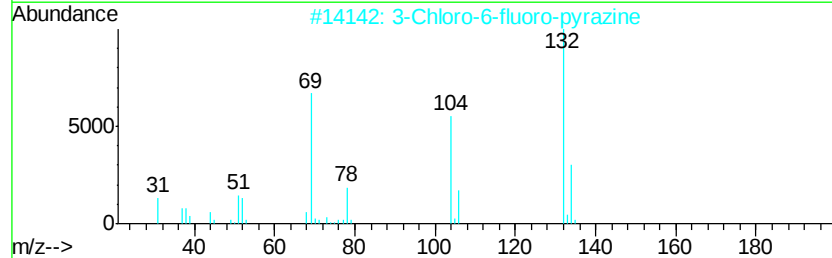
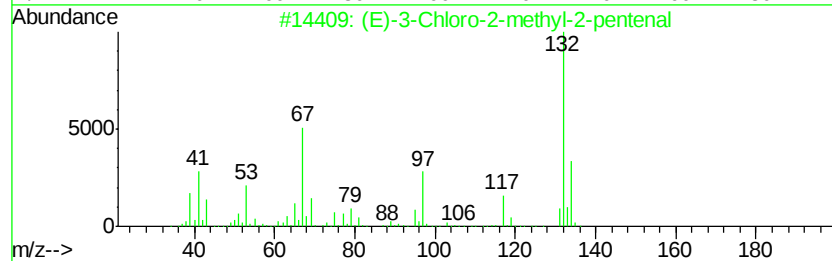
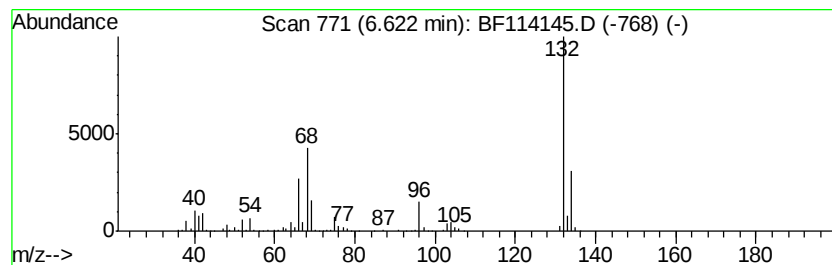
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown6.62 Concentration Rank 1

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 6.62 | 6.20 ng | 523813 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 27   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 3    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Amphetaminil                        | 250 | C17H18N2  | 017590-01-1  | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.M  
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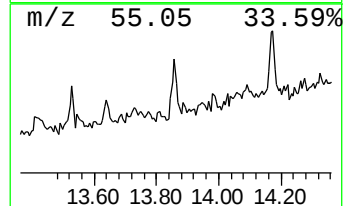
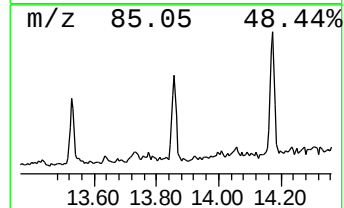
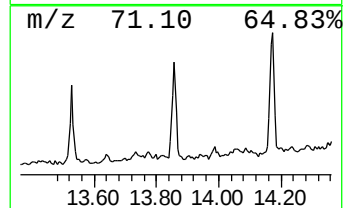
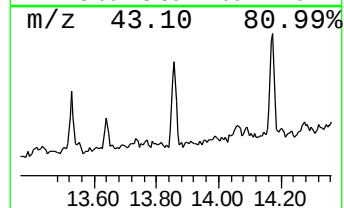
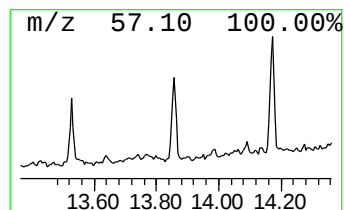
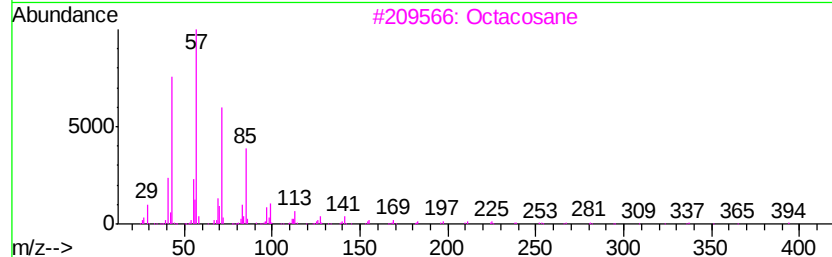
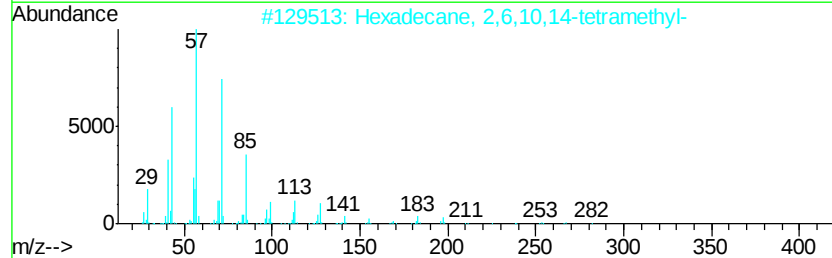
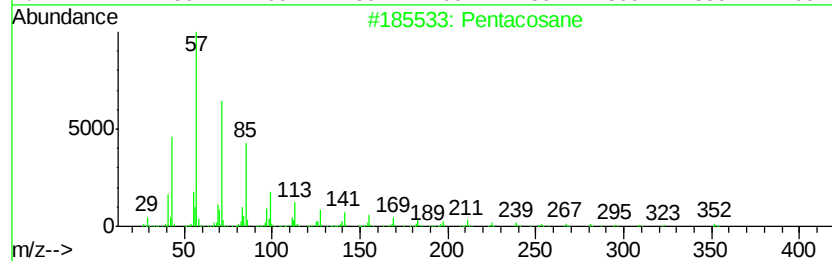
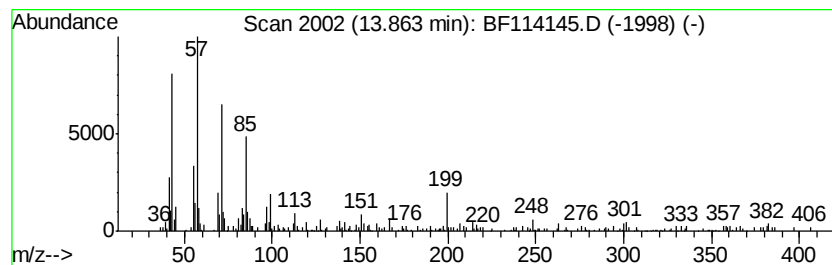
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Pentacosane Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.86 | 2.40 ng | 206341 | Chrysene-d12     | 14.01 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Pentacosane                        | 352 | C25H52  | 000629-99-2 | 93   |
| 2    |    | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42  | 000638-36-8 | 90   |
| 3    |    | Octacosane                         | 394 | C28H58  | 000630-02-4 | 90   |
| 4    |    | Octadecane, 3-methyl-              | 268 | C19H40  | 006561-44-0 | 87   |
| 5    |    | Docosane, 11-butyl-                | 366 | C26H54  | 013475-76-8 | 87   |



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ALS Vial : 23 Sample Multiplier: 1

Instrument :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.M  
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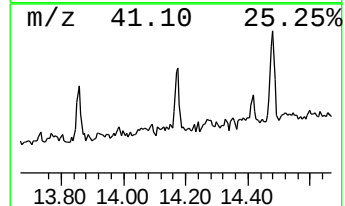
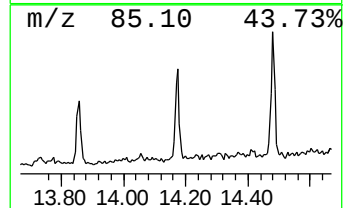
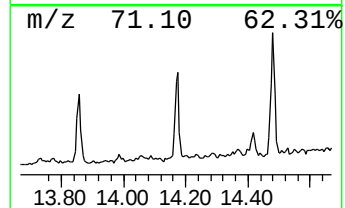
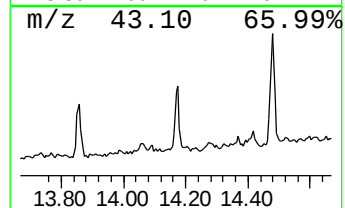
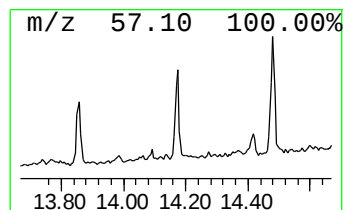
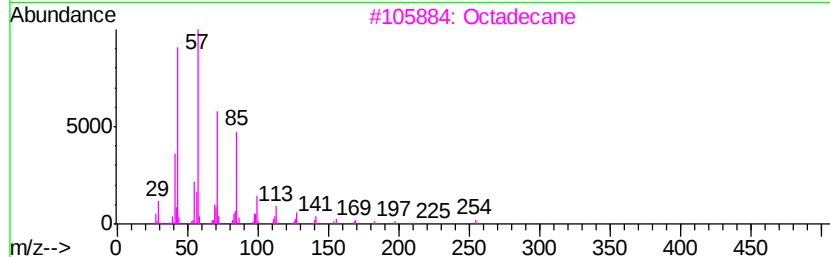
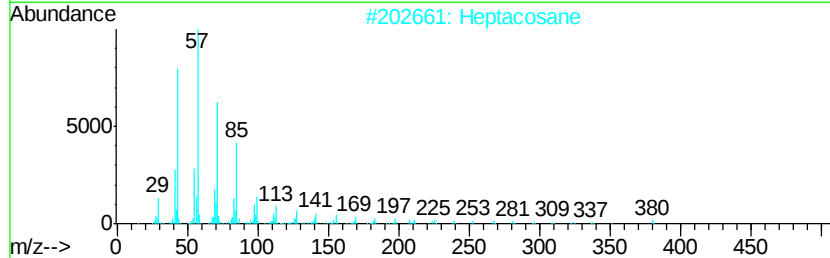
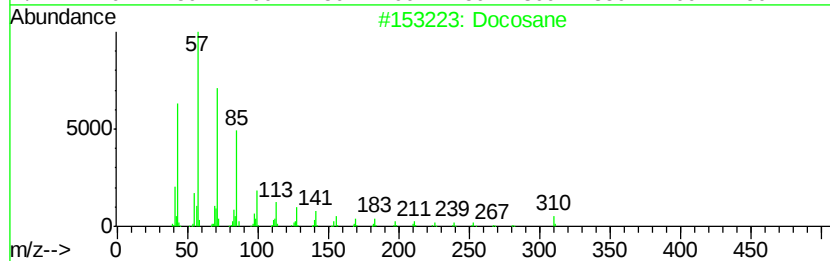
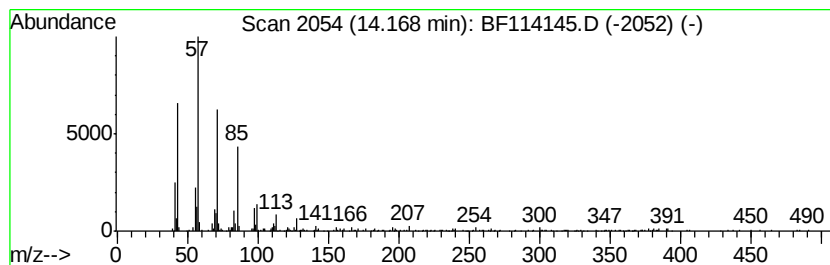
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Docosane Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.17 | 2.22 ng | 191070 | Chrysene-d12     | 14.01 |

| Hit# of | 5                      | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|------------------------|--------------|-----|---------|-------------|------|
| 1       | Docosane               |              | 310 | C22H46  | 000629-97-0 | 95   |
| 2       | Heptacosane            |              | 380 | C27H56  | 000593-49-7 | 95   |
| 3       | Octadecane             |              | 254 | C18H38  | 000593-45-3 | 91   |
| 4       | Heptadecane            |              | 240 | C17H36  | 000629-78-7 | 87   |
| 5       | Heptadecane, 2-methyl- |              | 254 | C18H38  | 001560-89-0 | 87   |



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ALS Vial : 23 Sample Multiplier: 1

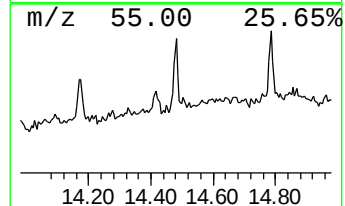
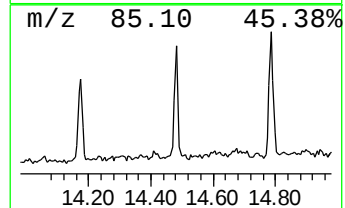
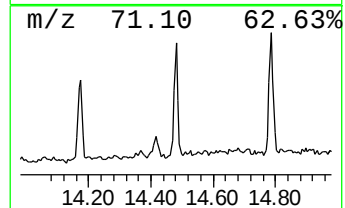
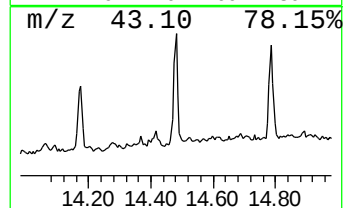
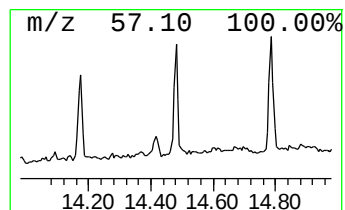
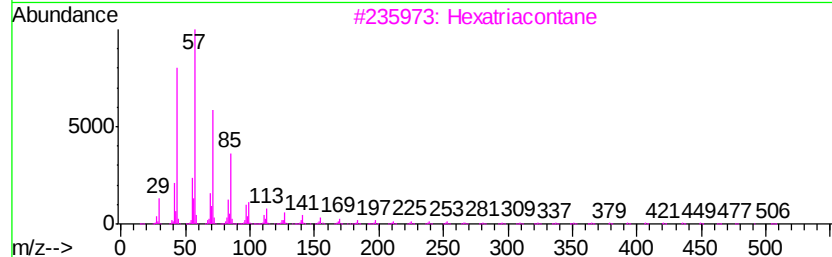
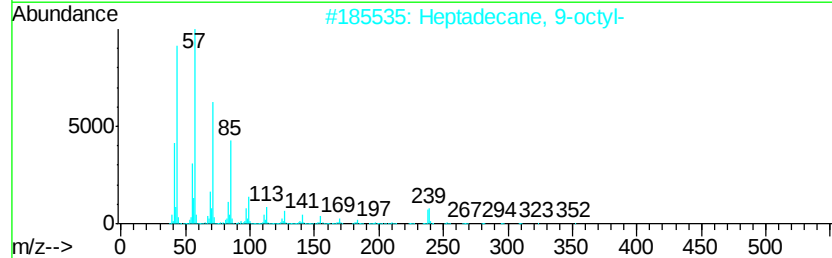
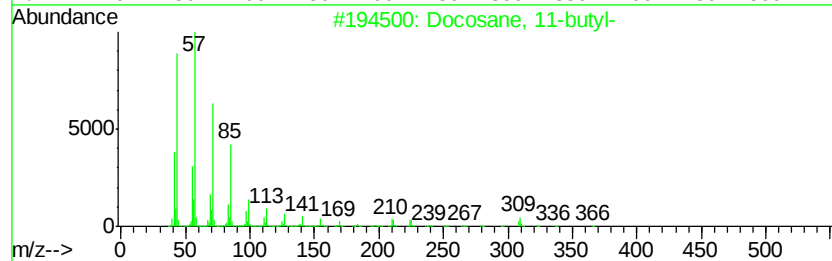
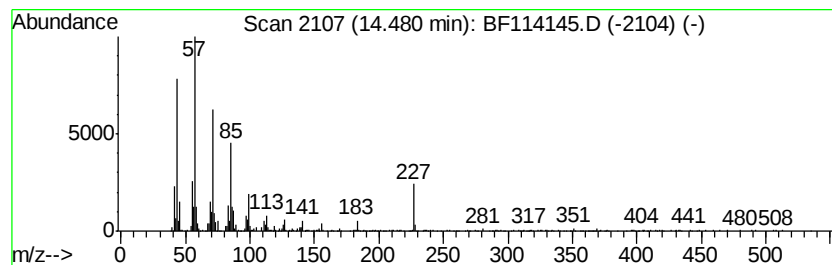
Instrument :  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Docosane, 11-butyl- Concentration Rank 5

| R.T.    | EstConc | Area                      | Relative to ISTD | R.T.           |
|---------|---------|---------------------------|------------------|----------------|
| 14.48   | 4.07 ng | 349855                    | Chrysene-d12     | 14.01          |
| Hit# of | 5       | Tentative ID              | MW MolForm       | CAS# Qual      |
| 1       |         | Docosane, 11-butyl-       | 366 C26H54       | 013475-76-8 89 |
| 2       |         | Heptadecane, 9-octyl-     | 352 C25H52       | 007225-64-1 87 |
| 3       |         | Hexatriacontane           | 507 C36H74       | 000630-06-8 84 |
| 4       |         | Octadecane, 5,14-dibutyl- | 366 C26H54       | 055282-13-8 78 |
| 5       |         | Eicosane, 10-methyl-      | 296 C21H44       | 054833-23-7 78 |



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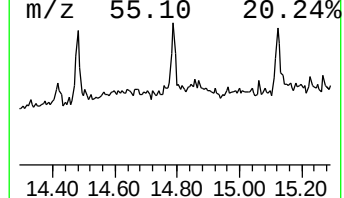
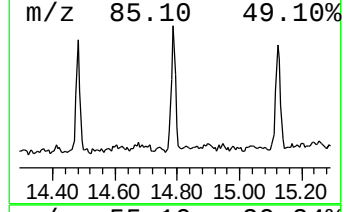
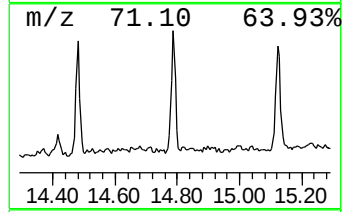
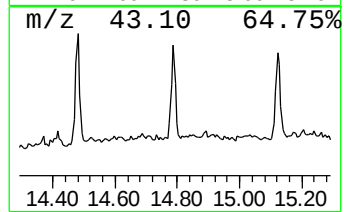
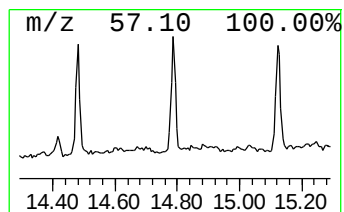
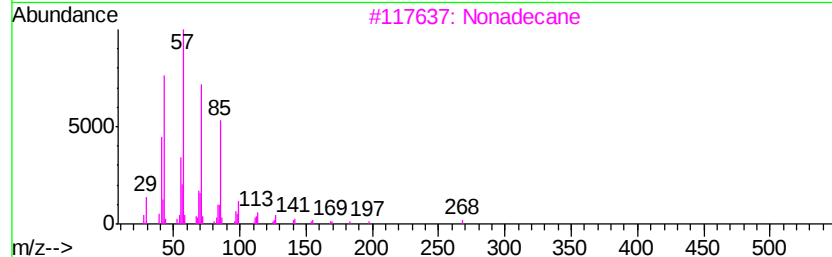
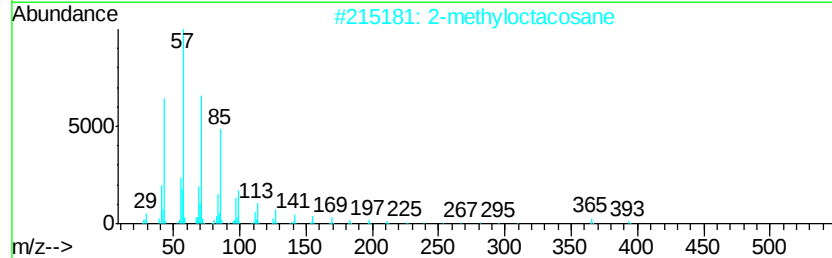
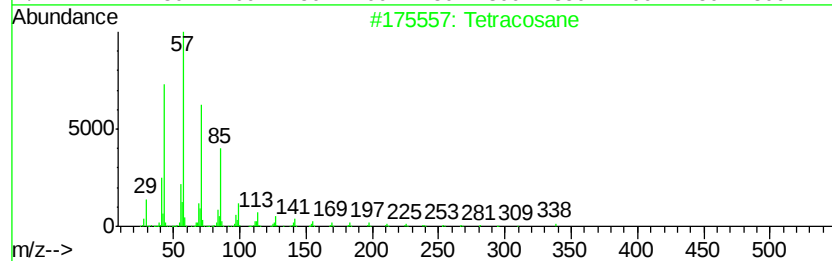
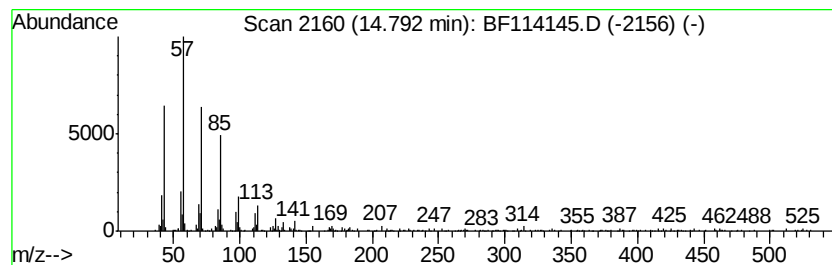
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Tetracosane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.79 | 3.59 ng | 294229 | Perylene-d12     | 15.48 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm | CAS#         | Qual |
|---------|---|---------------------|-----|---------|--------------|------|
| 1       |   | Tetracosane         | 338 | C24H50  | 000646-31-1  | 87   |
| 2       |   | 2-methyloctacosane  | 408 | C29H60  | 1000376-72-8 | 86   |
| 3       |   | Nonadecane          | 268 | C19H40  | 000629-92-5  | 86   |
| 4       |   | Heptadecane         | 240 | C17H36  | 000629-78-7  | 86   |
| 5       |   | Dodecane, 2-methyl- | 184 | C13H28  | 001560-97-0  | 81   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF051019\  
Data File : BF114145.D  
Acq On : 11 May 2019 2:18  
Operator : JU/SJ  
Sample : K2750-03 10X  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
72-11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

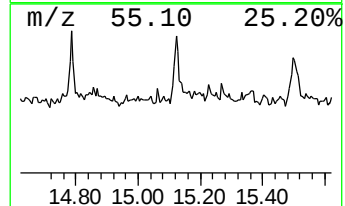
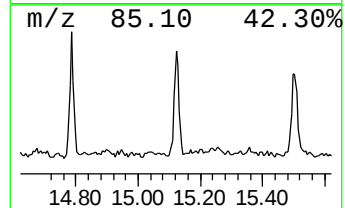
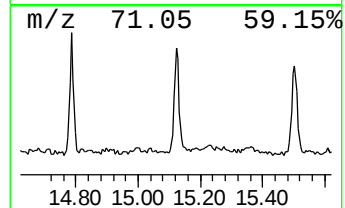
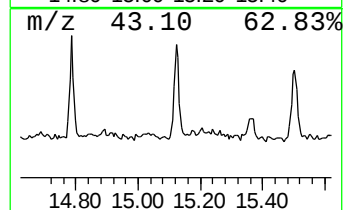
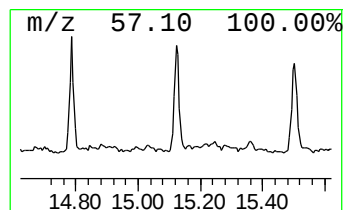
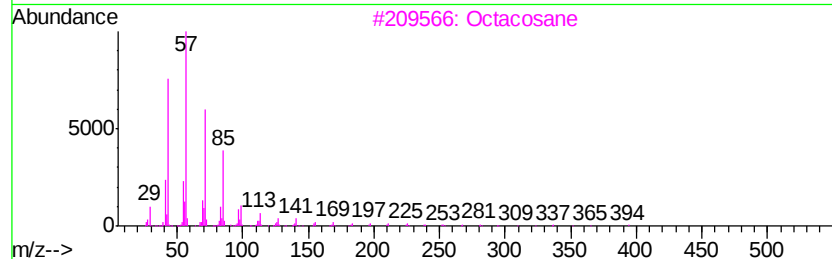
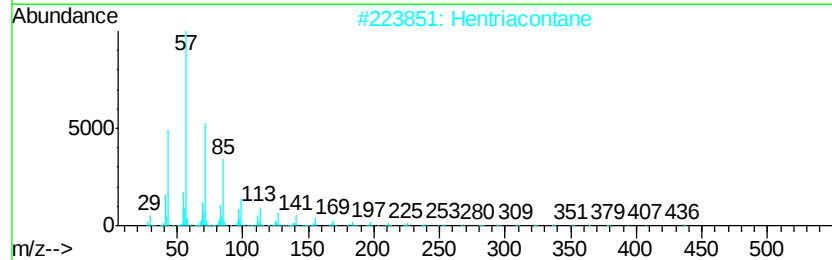
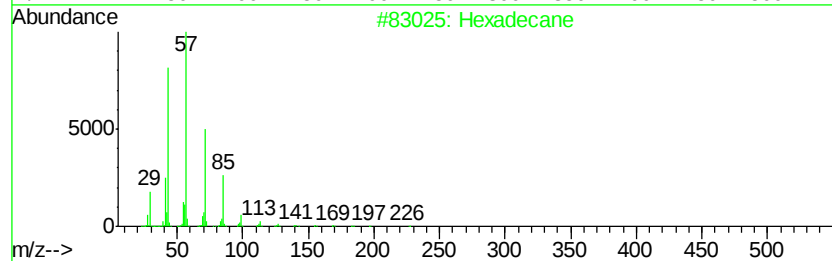
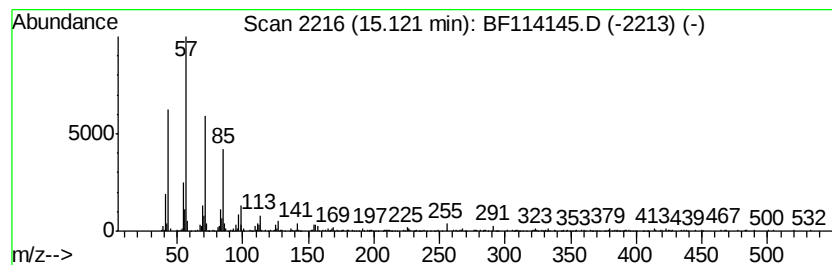
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Hexadecane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.12 | 4.13 ng | 337957 | Perylene-d12     | 15.48 |

| Hit# | of | Tentative ID       | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------|-----|---------|-------------|------|
| 1    | 5  | Hexadecane         | 226 | C16H34  | 000544-76-3 | 95   |
| 2    |    | Hentriacontane     | 437 | C31H64  | 000630-04-6 | 92   |
| 3    |    | Octacosane         | 394 | C28H58  | 000630-02-4 | 91   |
| 4    |    | Docosane, 9-octyl- | 422 | C30H62  | 055319-83-0 | 87   |
| 5    |    | Heptacosane        | 380 | C27H56  | 000593-49-7 | 87   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF051019\  
Data File : BF114145.D  
Acq On : 11 May 2019 2:18  
Operator : JU/SJ  
Sample : K2750-03 10X  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
72-11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

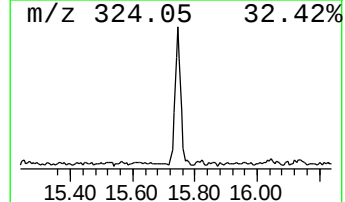
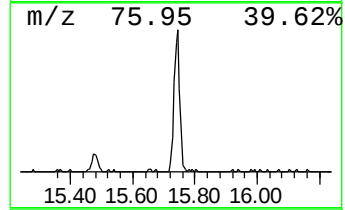
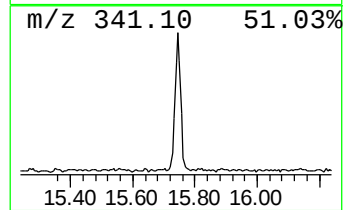
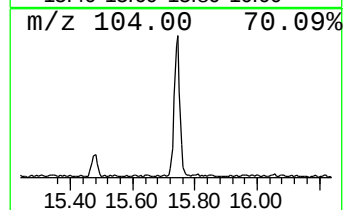
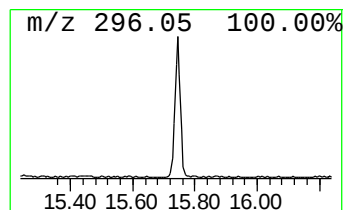
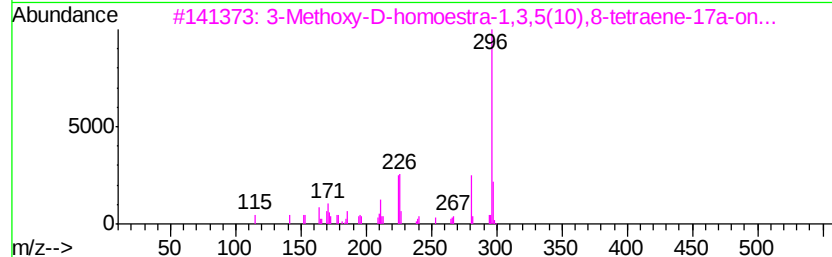
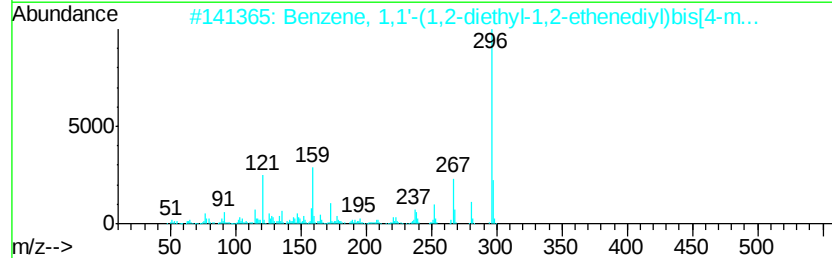
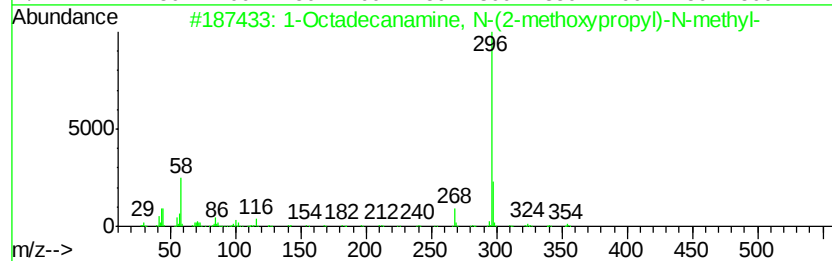
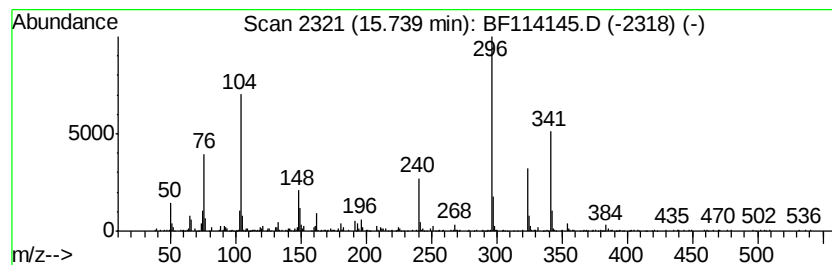
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 unknown15.74 Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.74 | 5.35 ng | 437987 | Perylene-d12     | 15.48 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | 1-Octadecanamine, N-(2-methoxypr... | 355 | C23H49NO   | 1000196-18-5 | 27   |
| 2    |    | Benzene, 1,1'-(1,2-diethyl-1,2-e... | 296 | C20H24O2   | 007773-34-4  | 27   |
| 3    |    | 3-Methoxy-D-homoestra-1,3,5(10),... | 296 | C20H24O2   | 002000-72-8  | 23   |
| 4    |    | 2-Thiazolamine, 4-(4-methoxyphen... | 296 | C17H16N2OS | 1000319-57-2 | 16   |
| 5    |    | 2-(2-Quinolyl)(1,2,4)triazolo(1,... | 296 | C19H12N4   | 1000241-15-8 | 16   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF051019\  
Data File : BF114145.D  
Acq On : 11 May 2019 2:18  
Operator : JU/SJ  
Sample : K2750-03 10X  
Misc :  
ALS Vial : 23 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
72-11995

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF051019.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 |
| unknown6.62         | 6.62  | 6.2     | ng    | 523813   | 1                     | 6.86  | 1688720 | 20.0 |
| Pentacosane         | 13.86 | 2.4     | ng    | 206341   | 5                     | 14.01 | 1719570 | 20.0 |
| Docosane            | 14.17 | 2.2     | ng    | 191070   | 5                     | 14.01 | 1719570 | 20.0 |
| Docosane, 11-butyl- | 14.48 | 4.1     | ng    | 349855   | 5                     | 14.01 | 1719570 | 20.0 |
| Tetracosane         | 14.79 | 3.6     | ng    | 294229   | 6                     | 15.48 | 1637380 | 20.0 |
| Hexadecane          | 15.12 | 4.1     | ng    | 337957   | 6                     | 15.48 | 1637380 | 20.0 |
| unknown15.74        | 15.74 | 5.3     | ng    | 437987   | 6                     | 15.48 | 1637380 | 20.0 |