

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\  
 Data File : BF109224.D  
 Acq On : 22 Sep 2018 16:34  
 Operator : JU/SJ  
 Sample : J5023-01  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 NB-PIT-1

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-BF092218.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         | 4.887       | 473           | 476         | 484          | rVB      | 39362          | 45756         | 3.08%           | 0.285%        |
| 2         | 5.310       | 543           | 548         | 551          | rBV      | 1368287        | 1236247       | 83.24%          | 7.691%        |
| 3         | 6.334       | 718           | 722         | 731          | rBV      | 1465142        | 1351586       | 91.01%          | 8.408%        |
| 4         | 6.469       | 741           | 745         | 748          | rBV      | 1557872        | 1326653       | 89.33%          | 8.253%        |
| 5         | 6.704       | 781           | 785         | 788          | rBV      | 766987         | 613775        | 41.33%          | 3.818%        |
| 6         | 6.857       | 808           | 811         | 815          | rBV      | 1124708        | 1008619       | 67.92%          | 6.275%        |
| 7         | 7.263       | 875           | 880         | 883          | rBV      | 940752         | 801666        | 53.98%          | 4.987%        |
| 8         | 7.986       | 999           | 1003        | 1006         | rBV      | 949101         | 802602        | 54.04%          | 4.993%        |
| 9         | 9.063       | 1181          | 1186        | 1189         | rBV      | 1650513        | 1485094       | 100.00%         | 9.239%        |
| 10        | 9.457       | 1249          | 1253        | 1256         | rBV      | 468392         | 419956        | 28.28%          | 2.613%        |
| 11        | 9.733       | 1296          | 1300        | 1304         | rVB2     | 1099805        | 911480        | 61.38%          | 5.670%        |
| 12        | 10.516      | 1429          | 1433        | 1440         | rBV      | 1063801        | 911837        | 61.40%          | 5.672%        |
| 13        | 11.210      | 1547          | 1551        | 1554         | rBV      | 1187047        | 960564        | 64.68%          | 5.976%        |
| 14        | 11.751      | 1640          | 1643        | 1646         | rBV2     | 18295          | 19402         | 1.31%           | 0.121%        |
| 15        | 12.792      | 1816          | 1820        | 1823         | rBV      | 1726766        | 1472414       | 99.15%          | 9.160%        |
| 16        | 13.704      | 1971          | 1975        | 1993         | rBV      | 89052          | 182165        | 12.27%          | 1.133%        |
| 17        | 13.833      | 1993          | 1997        | 2000         | rBV      | 963298         | 844324        | 56.85%          | 5.252%        |
| 18        | 14.021      | 2025          | 2029        | 2032         | rBV      | 22931          | 20236         | 1.36%           | 0.126%        |
| 19        | 14.321      | 2077          | 2080        | 2083         | rBV      | 45575          | 43509         | 2.93%           | 0.271%        |
| 20        | 14.615      | 2126          | 2130        | 2137         | rVB      | 82261          | 82830         | 5.58%           | 0.515%        |
| 21        | 14.933      | 2179          | 2184        | 2189         | rBV      | 140205         | 160041        | 10.78%          | 0.996%        |
| 22        | 15.227      | 2229          | 2234        | 2239         | rBV      | 527626         | 593615        | 39.97%          | 3.693%        |
| 23        | 15.286      | 2239          | 2244        | 2256         | rVB      | 195923         | 260375        | 17.53%          | 1.620%        |
| 24        | 15.686      | 2305          | 2312        | 2321         | rBV      | 176957         | 261659        | 17.62%          | 1.628%        |
| 25        | 16.145      | 2382          | 2390        | 2399         | rBV      | 98358          | 170835        | 11.50%          | 1.063%        |
| 26        | 16.686      | 2475          | 2482        | 2489         | rBV      | 32629          | 65768         | 4.43%           | 0.409%        |
| 27        | 17.321      | 2583          | 2590        | 2596         | rVB5     | 9495           | 21833         | 1.47%           | 0.136%        |

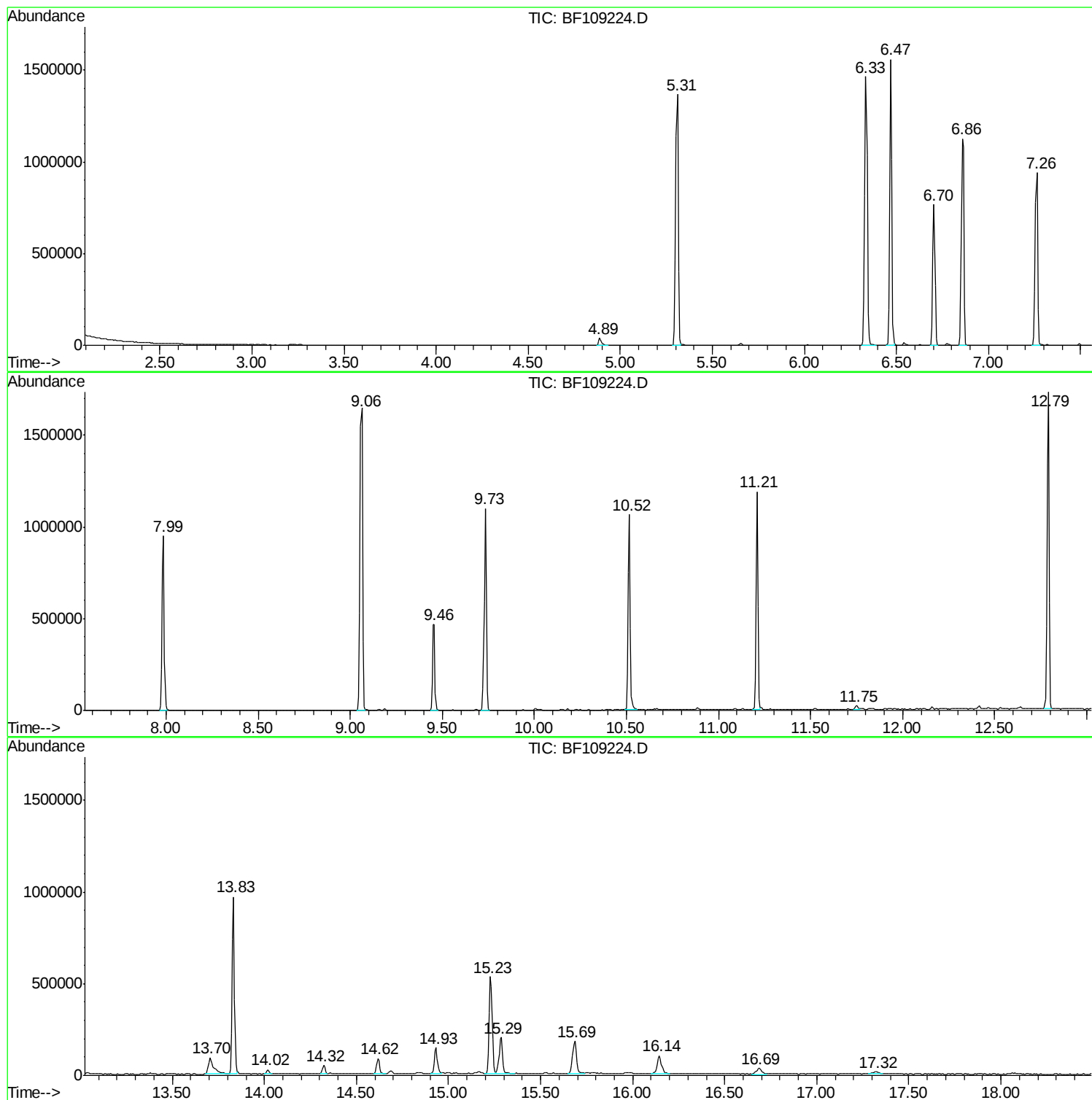
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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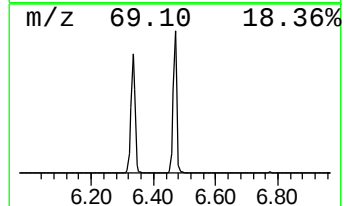
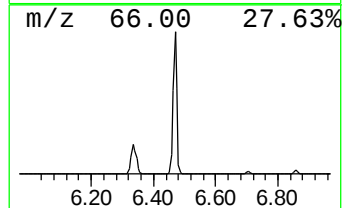
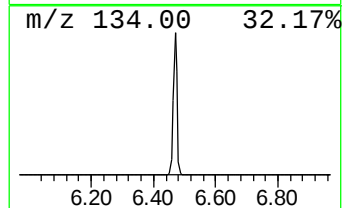
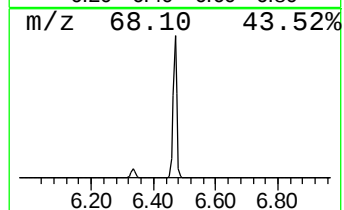
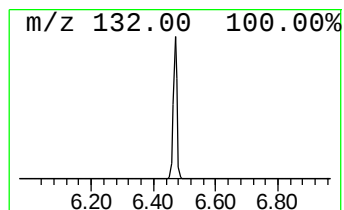
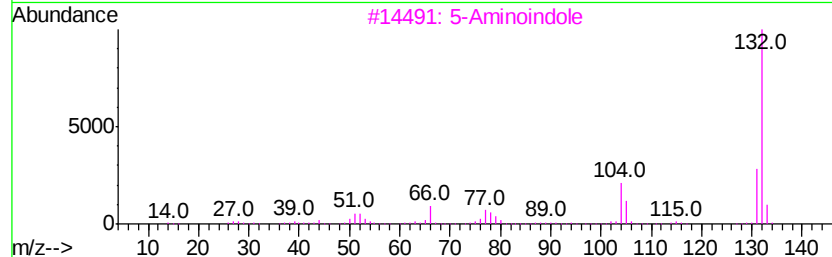
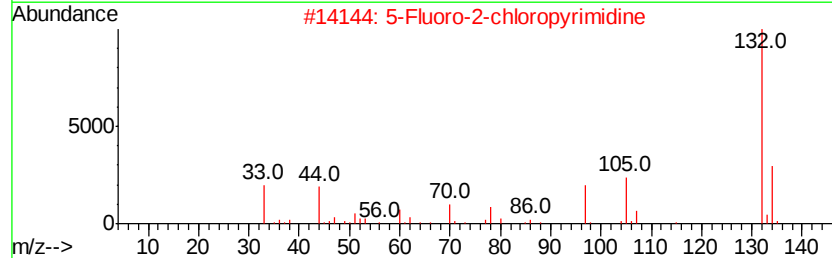
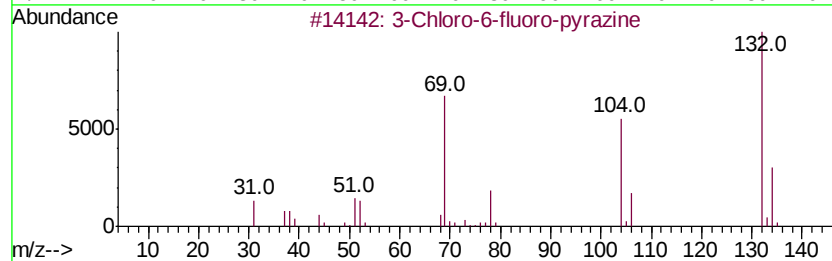
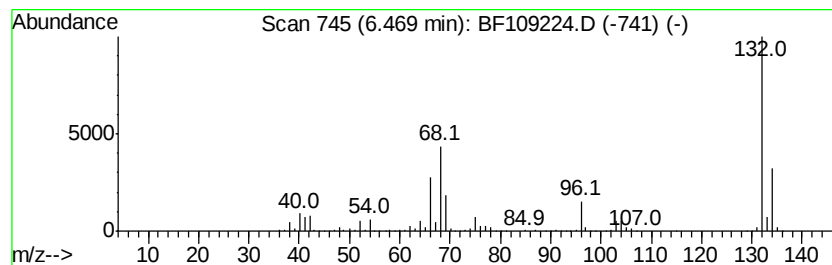
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.47 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.47 | 43.23 ng | 1326650 | 1,4-Dichlorobenzene-d4 | 6.70 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



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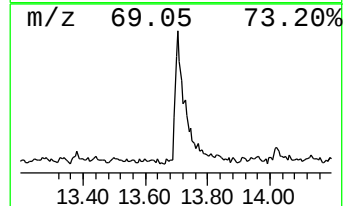
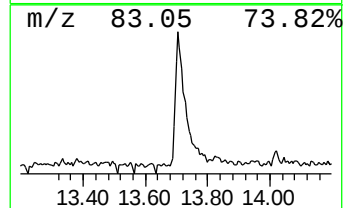
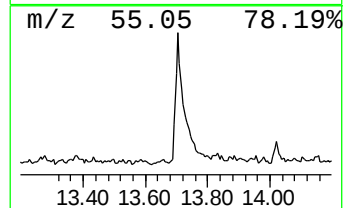
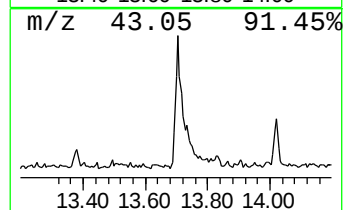
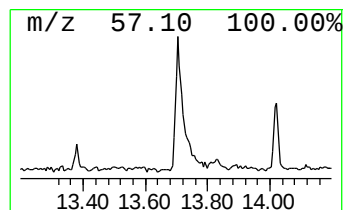
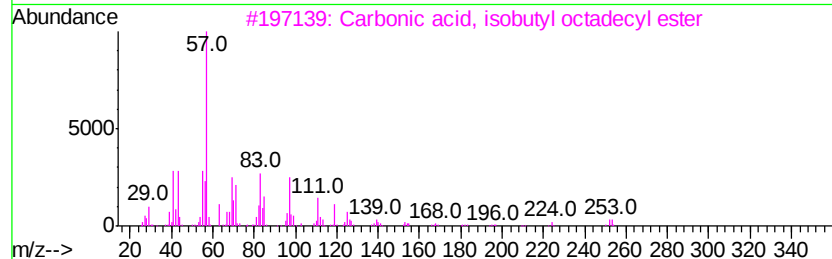
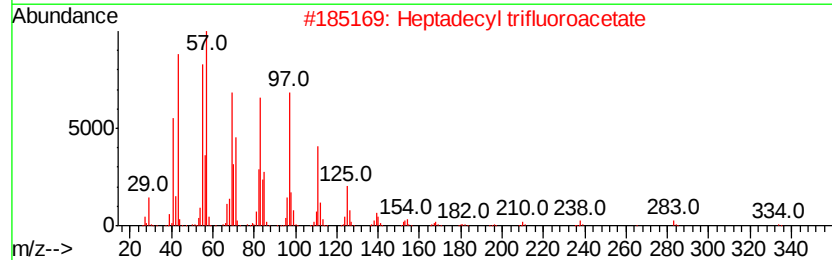
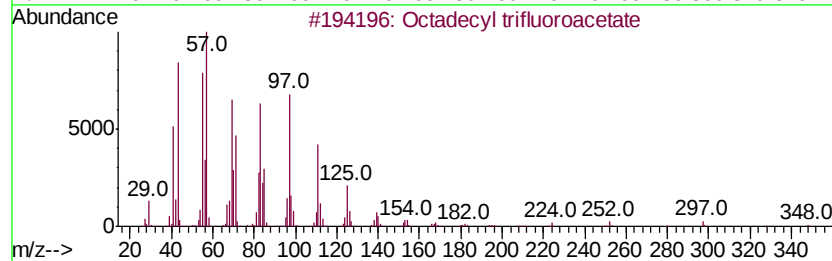
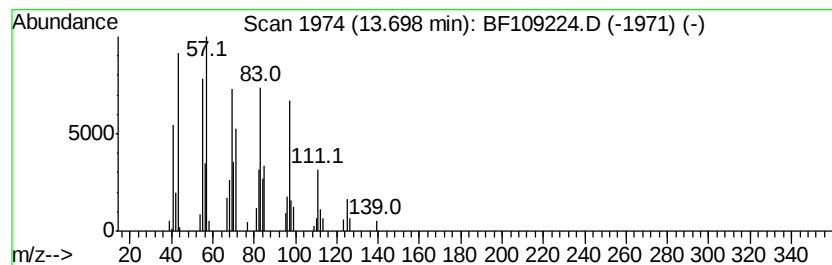
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Octadecyl trifluoroacetate Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.70 | 4.32 ng | 182165 | Chrysene-d12     | 13.83 |

| Hit# of | 5                       | Tentative ID         | MW  | MolForm    | CAS#         | Qual |
|---------|-------------------------|----------------------|-----|------------|--------------|------|
| 1       | Octadecyl               | trifluoroacetate     | 366 | C20H37F3O2 | 079392-43-1  | 91   |
| 2       | Heptadecyl              | trifluoroacetate     | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 3       | Carbonic acid, isobutyl | octadecyl...         | 370 | C23H46O3   | 1000314-61-5 | 91   |
| 4       | 17-Pentatriacontene     |                      | 491 | C35H70     | 006971-40-0  | 90   |
| 5       | Isobutyl                | tetradecyl carbonate | 314 | C19H38O3   | 959275-58-2  | 90   |



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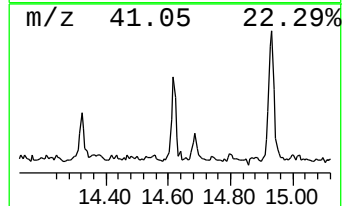
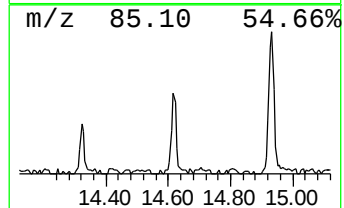
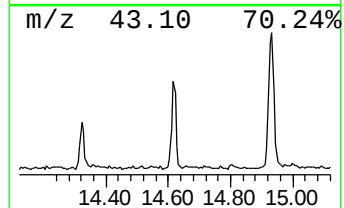
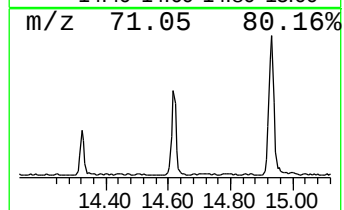
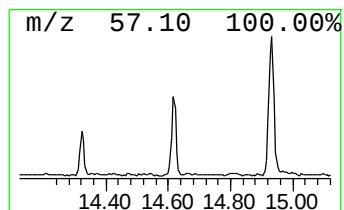
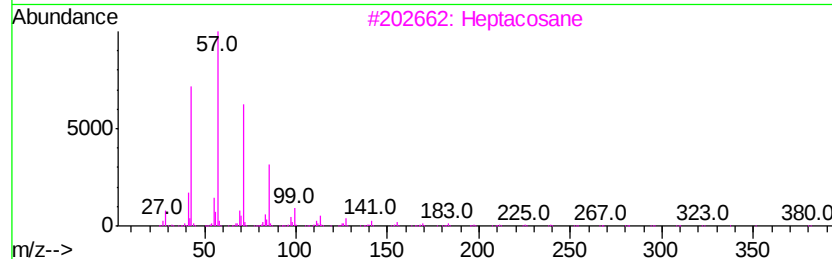
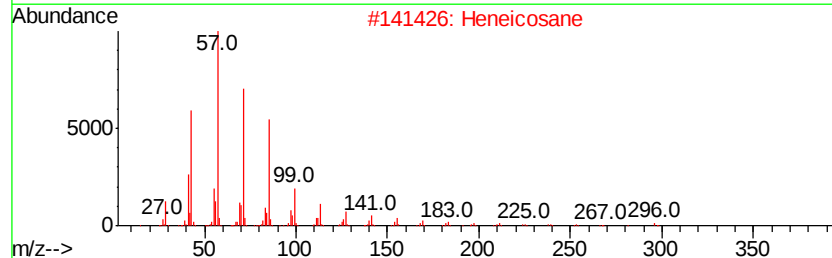
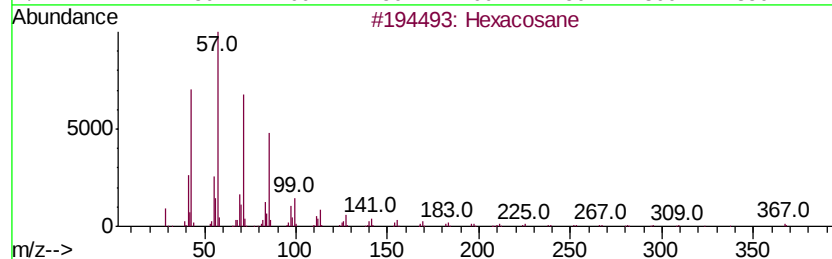
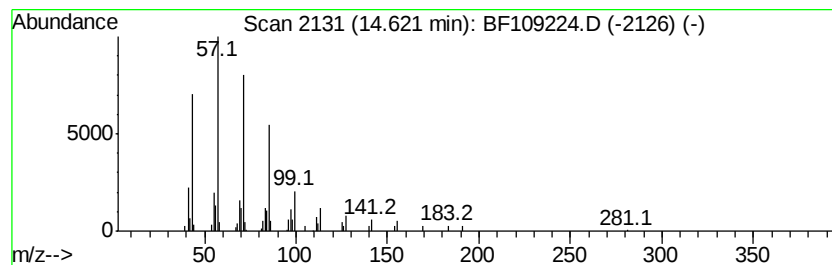
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Hexacosane Concentration Rank 8

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.62 | 2.79 ng | 82830 | Perylene-d12     | 15.23 |

| Hit# of | 5           | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|-------------|--------------|-----|---------|-------------|------|
| 1       | Hexacosane  |              | 366 | C26H54  | 000630-01-3 | 91   |
| 2       | Heneicosane |              | 296 | C21H44  | 000629-94-7 | 91   |
| 3       | Heptacosane |              | 380 | C27H56  | 000593-49-7 | 91   |
| 4       | Triacontane |              | 422 | C30H62  | 000638-68-6 | 91   |
| 5       | Tetracosane |              | 338 | C24H50  | 000646-31-1 | 90   |



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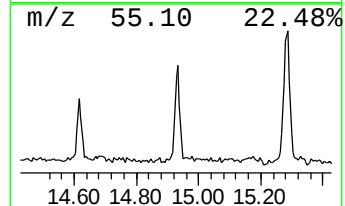
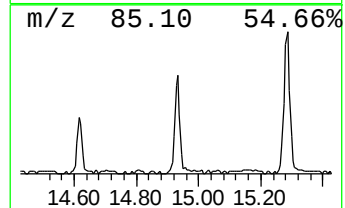
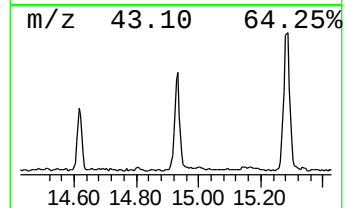
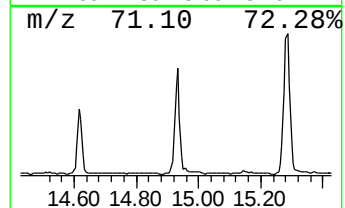
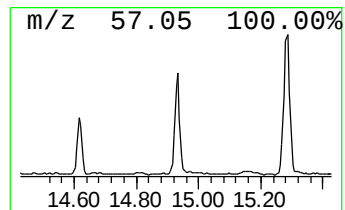
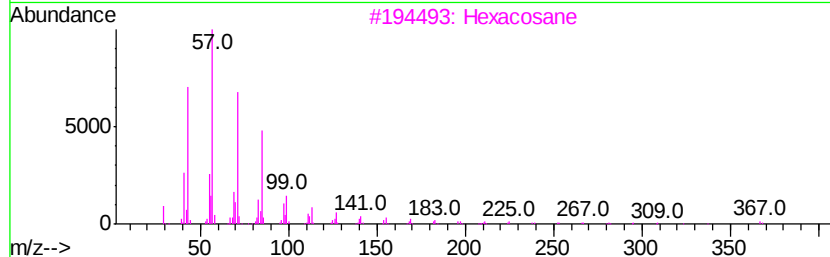
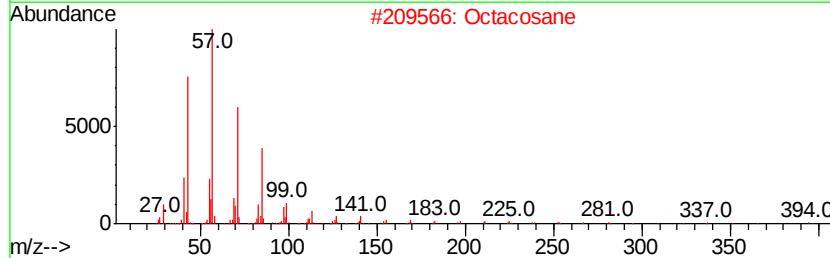
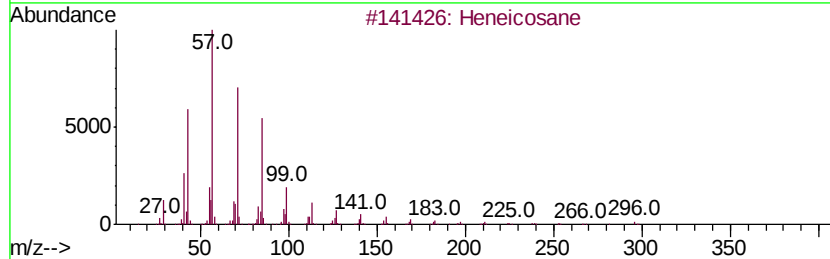
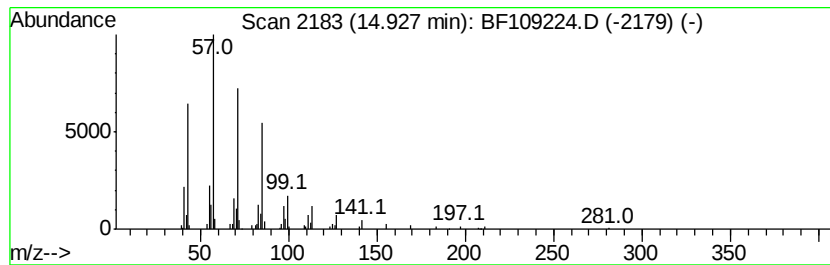
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ClientSampleId :  
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Peak Number 5 Heneicosane Concentration Rank 6

| R.T.      | EstConc               | Area   | Relative to ISTD | R.T.         |      |
|-----------|-----------------------|--------|------------------|--------------|------|
| 14.93     | 5.39 ng               | 160041 | Perylene-d12     | 15.23        |      |
| Hit# of 5 | Tentative ID          | MW     | MolForm          | CAS#         | Qual |
| 1         | Heneicosane           | 296    | C21H44           | 000629-94-7  | 91   |
| 2         | Octacosane            | 394    | C28H58           | 000630-02-4  | 90   |
| 3         | Hexacosane            | 366    | C26H54           | 000630-01-3  | 90   |
| 4         | Nonadecane, 2-methyl- | 282    | C20H42           | 001560-86-7  | 90   |
| 5         | 6,6-Diethylhexadecane | 282    | C20H42           | 1000360-41-4 | 90   |



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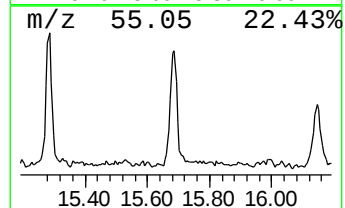
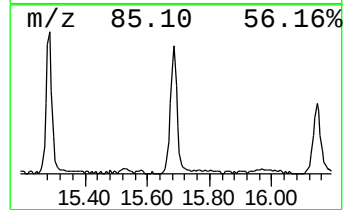
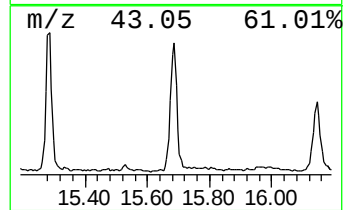
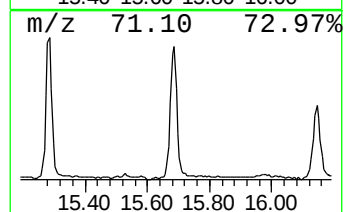
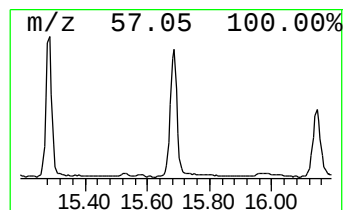
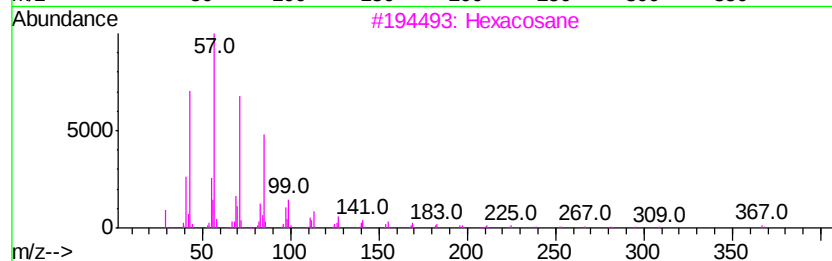
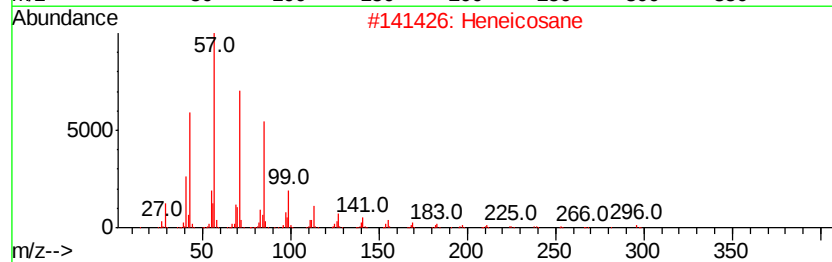
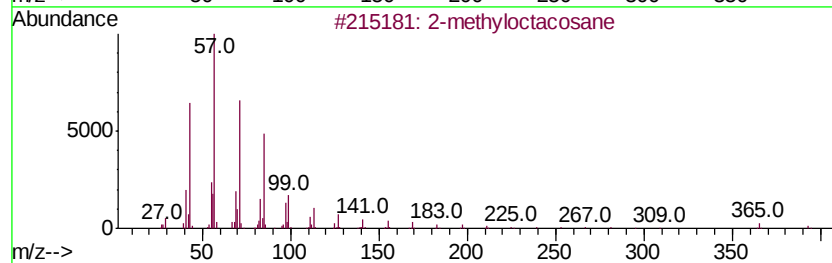
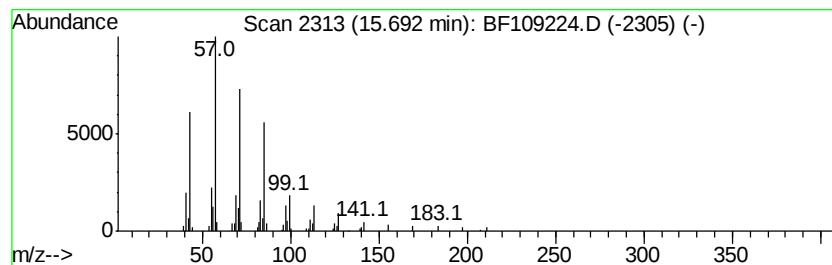
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 2-methyloctacosane Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.69 | 8.82 ng | 261659 | Perylene-d12     | 15.23 |

| Hit# | of | Tentative ID                     | MW  | MolForm | CAS#         | Qual |
|------|----|----------------------------------|-----|---------|--------------|------|
| 1    | 5  | 2-methyloctacosane               | 408 | C29H60  | 1000376-72-8 | 91   |
| 2    |    | Heneicosane                      | 296 | C21H44  | 000629-94-7  | 91   |
| 3    |    | Hexacosane                       | 366 | C26H54  | 000630-01-3  | 91   |
| 4    |    | Octacosane                       | 394 | C28H58  | 000630-02-4  | 91   |
| 5    |    | Heneicosane, 11-(1-ethylpropyl)- | 366 | C26H54  | 055282-11-6  | 91   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF092218\  
Data File : BF109224.D  
Acq On : 22 Sep 2018 16:34  
Operator : JU/SJ  
Sample : J5023-01  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
NB-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

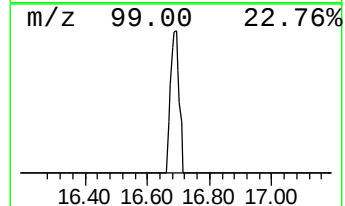
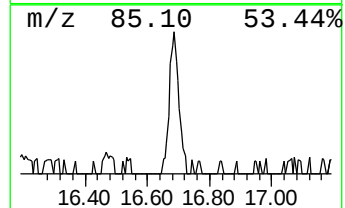
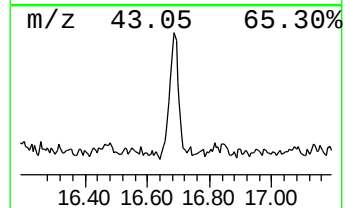
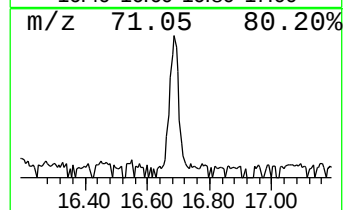
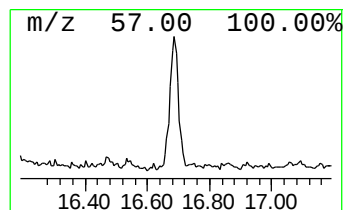
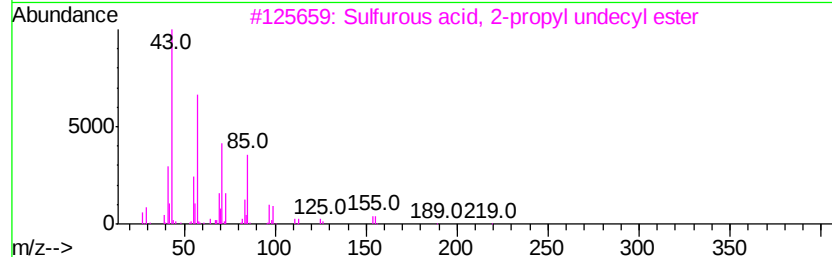
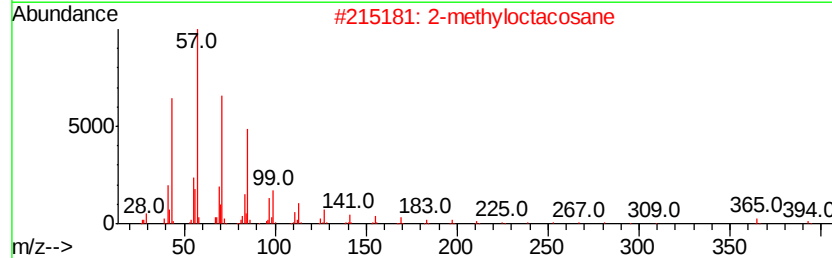
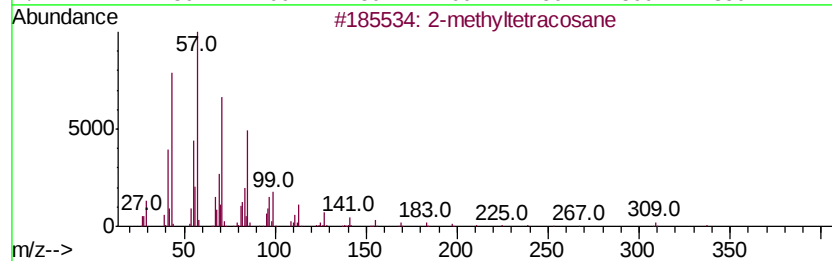
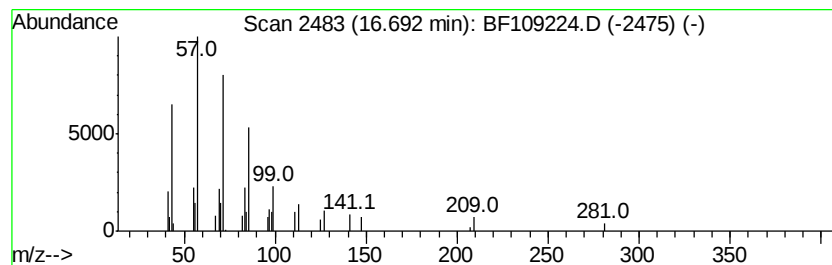
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 9 2-methyltetracosane Concentration Rank 9

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 16.69 | 2.22 ng | 65768 | Perylene-d12     | 15.23 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 2-methyltetracosane                 | 352 | C25H52    | 1000376-72-6 | 90   |
| 2    |    | 2-methyloctacosane                  | 408 | C29H60    | 1000376-72-8 | 90   |
| 3    |    | Sulfurous acid, 2-propyl undecyl... | 278 | C14H30O3S | 1000309-12-2 | 86   |
| 4    |    | Hexacosane                          | 366 | C26H54    | 000630-01-3  | 86   |
| 5    |    | Heneicosane, 11-(1-ethylpropyl)-    | 366 | C26H54    | 055282-11-6  | 86   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF092218\  
Data File : BF109224.D  
Acq On : 22 Sep 2018 16:34  
Operator : JU/SJ  
Sample : J5023-01  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
NB-PIT-1

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF092218.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 |
| unknown6.47          | 6.47  | 43.2    | ng    | 1326650  | 1                     | 6.70  | 613775 | 20.0 |
| Octadecyl trifluo... | 13.70 | 4.3     | ng    | 182165   | 5                     | 13.83 | 844324 | 20.0 |
| Hexacosane           | 14.62 | 2.8     | ng    | 82830    | 6                     | 15.23 | 593615 | 20.0 |
| Heneicosane          | 14.93 | 5.4     | ng    | 160041   | 6                     | 15.23 | 593615 | 20.0 |
| 2-methyloctacosane   | 15.69 | 8.8     | ng    | 261659   | 6                     | 15.23 | 593615 | 20.0 |
| 2-methyltetracosane  | 16.69 | 2.2     | ng    | 65768    | 6                     | 15.23 | 593615 | 20.0 |