

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM072220\  
 Data File : BM026834.D  
 Acq On : 22 Jul 2020 16:12  
 Operator : JU/CG  
 Sample : L3370-07  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 TP-3-D

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\_M\METHODS\8270-BM070820.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         | 4.943       | 369           | 375         | 392          | rBV      | 1291021        | 1766435       | 44.30%          | 8.808%        |
| 2         | 6.513       | 636           | 642         | 658          | rBV      | 1290351        | 1923199       | 48.23%          | 9.590%        |
| 3         | 7.295       | 769           | 775         | 789          | rBV      | 298027         | 454862        | 11.41%          | 2.268%        |
| 4         | 8.448       | 964           | 971         | 983          | rBV      | 712150         | 1173509       | 29.43%          | 5.852%        |
| 5         | 10.054      | 1236          | 1244        | 1258         | rBV      | 340008         | 597613        | 14.99%          | 2.980%        |
| 6         | 12.566      | 1664          | 1671        | 1687         | rBV      | 1573452        | 2250794       | 56.44%          | 11.224%       |
| 7         | 13.442      | 1814          | 1820        | 1829         | rBV      | 172135         | 250504        | 6.28%           | 1.249%        |
| 8         | 13.960      | 1902          | 1908        | 1921         | rVB      | 571456         | 805254        | 20.19%          | 4.015%        |
| 9         | 15.471      | 2159          | 2165        | 2183         | rBV      | 1538502        | 2104025       | 52.76%          | 10.492%       |
| 10        | 16.724      | 2369          | 2378        | 2390         | rBV      | 691005         | 989510        | 24.81%          | 4.934%        |
| 11        | 17.665      | 2533          | 2538        | 2546         | rBV      | 115707         | 171214        | 4.29%           | 0.854%        |
| 12        | 18.406      | 2659          | 2664        | 2669         | rBV      | 176660         | 218233        | 5.47%           | 1.088%        |
| 13        | 18.824      | 2731          | 2735        | 2745         | rBV      | 32096          | 47131         | 1.18%           | 0.235%        |
| 14        | 19.389      | 2825          | 2831        | 2838         | rBV      | 3429232        | 3987883       | 100.00%         | 19.886%       |
| 15        | 20.089      | 2946          | 2950        | 2956         | rVB      | 42491          | 55480         | 1.39%           | 0.277%        |
| 16        | 20.300      | 2981          | 2986        | 2991         | rBV      | 236051         | 283022        | 7.10%           | 1.411%        |
| 17        | 20.348      | 2991          | 2994        | 2998         | rVB      | 43769          | 46119         | 1.16%           | 0.230%        |
| 18        | 20.700      | 3049          | 3054        | 3064         | rBV      | 360970         | 537740        | 13.48%          | 2.681%        |
| 19        | 20.947      | 3091          | 3096        | 3106         | rBV      | 829933         | 1105087       | 27.71%          | 5.511%        |
| 20        | 21.142      | 3126          | 3129        | 3133         | rBV      | 41285          | 49248         | 1.23%           | 0.246%        |
| 21        | 21.559      | 3197          | 3200        | 3209         | rBV5     | 48330          | 100636        | 2.52%           | 0.502%        |
| 22        | 22.441      | 3347          | 3350        | 3354         | rVB2     | 47812          | 47573         | 1.19%           | 0.237%        |
| 23        | 23.018      | 3442          | 3448        | 3456         | rBV      | 573167         | 977084        | 24.50%          | 4.872%        |
| 24        | 23.588      | 3542          | 3545        | 3554         | rVB4     | 58514          | 111760        | 2.80%           | 0.557%        |

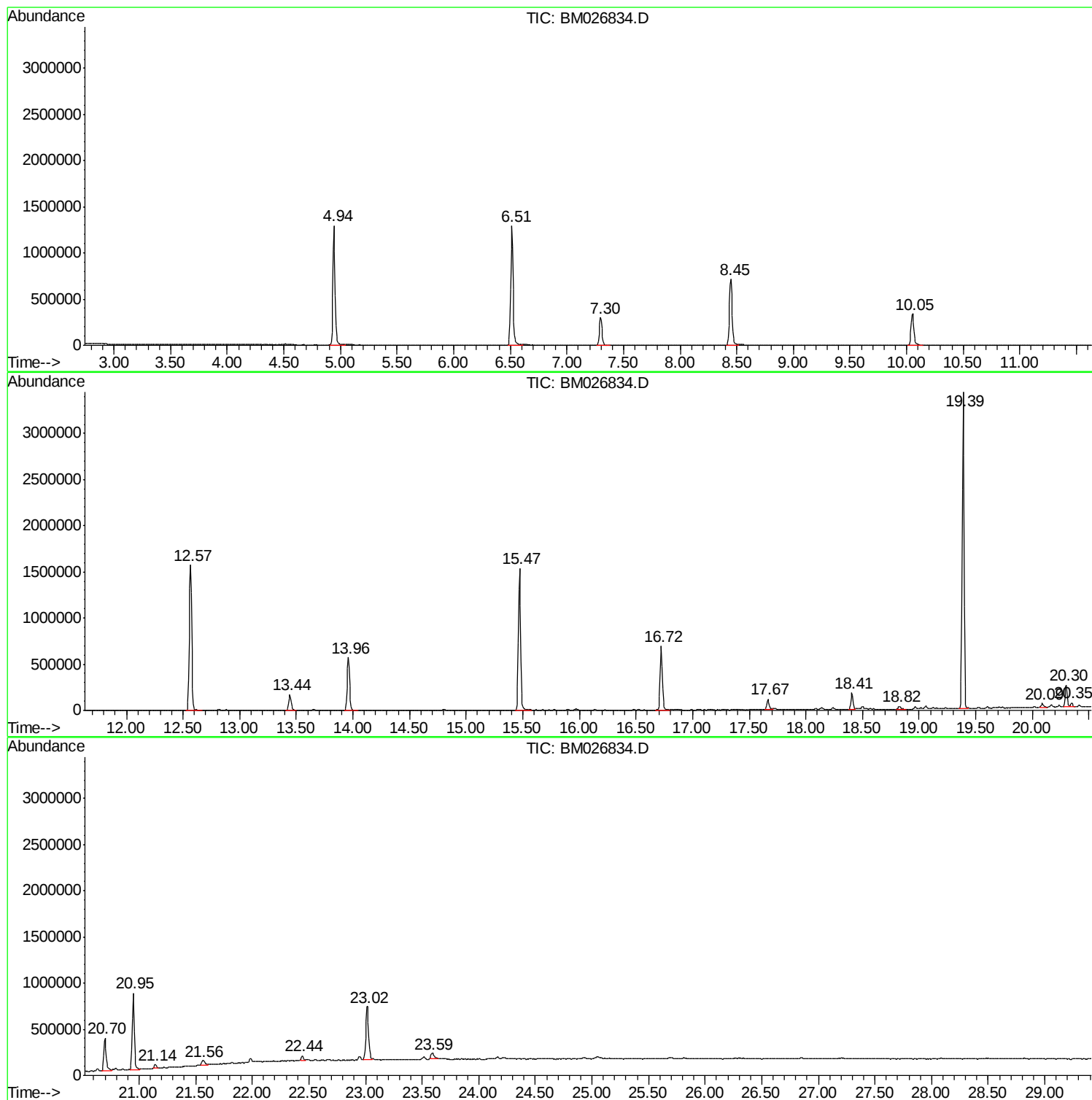
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Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
TP-3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070820.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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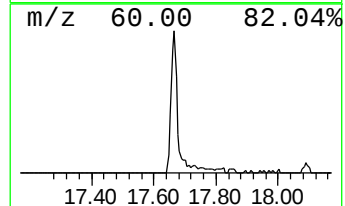
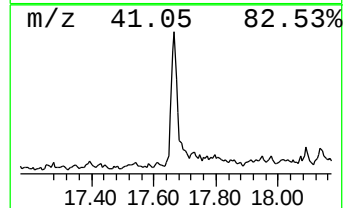
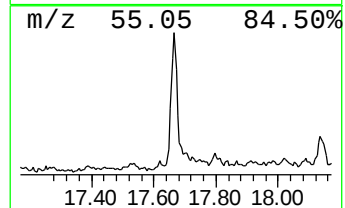
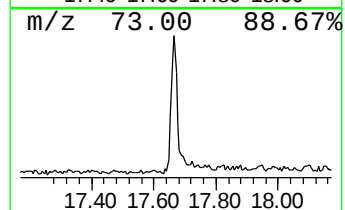
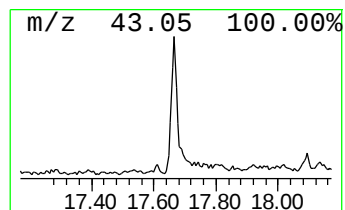
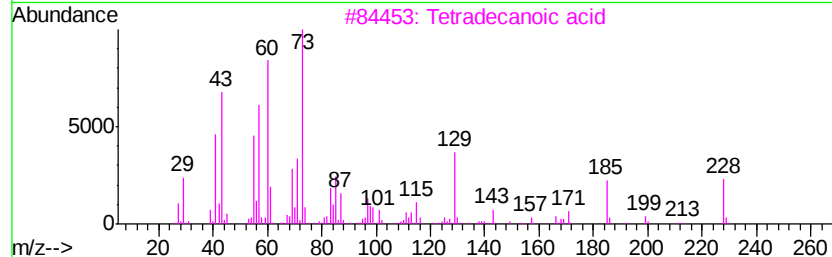
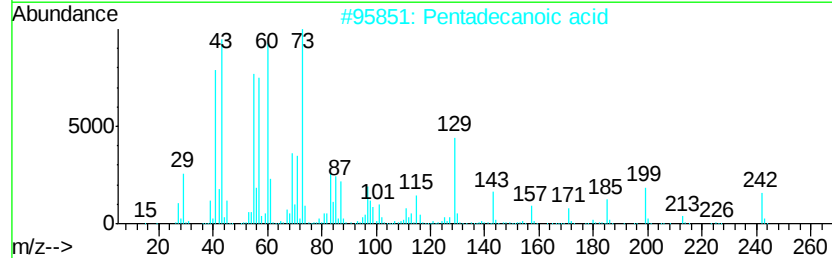
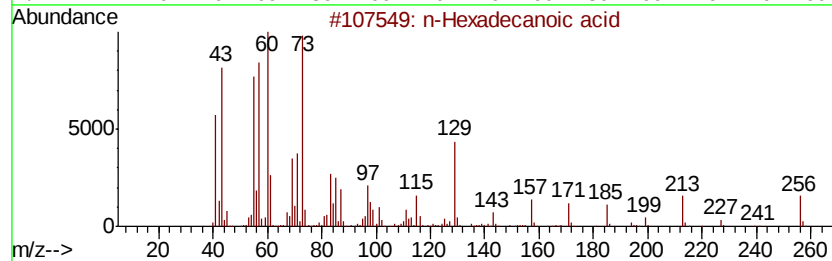
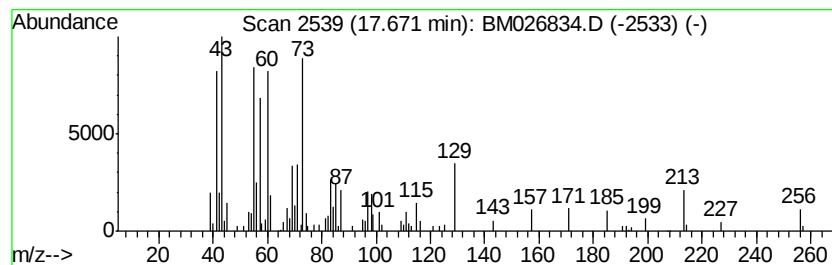
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 17.67 | 3.46 ng | 171214 | Phenanthrene-d10 | 16.72 |

| 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 | 81   |
| 3       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |
| 4       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 70   |
| 5       |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 59   |



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Instrument :  
BNA\_M  
ClientSampleId :  
TP-3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070820.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

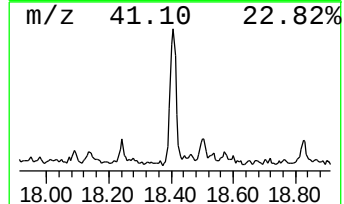
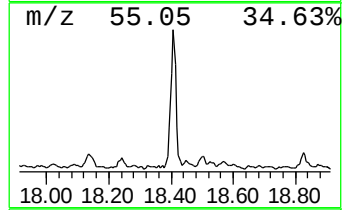
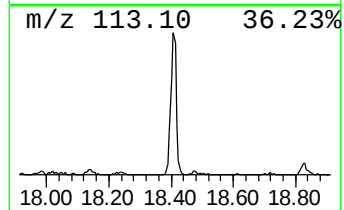
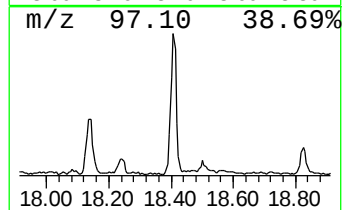
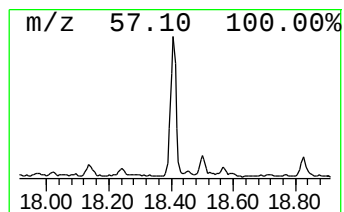
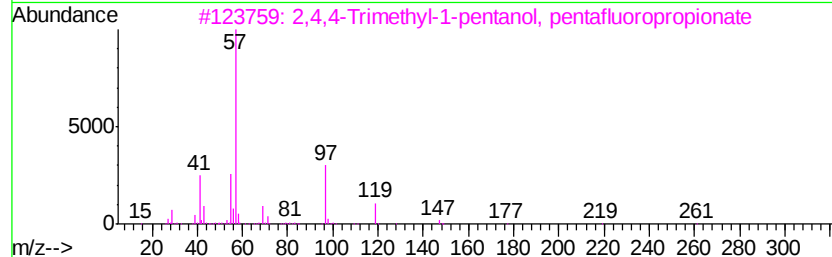
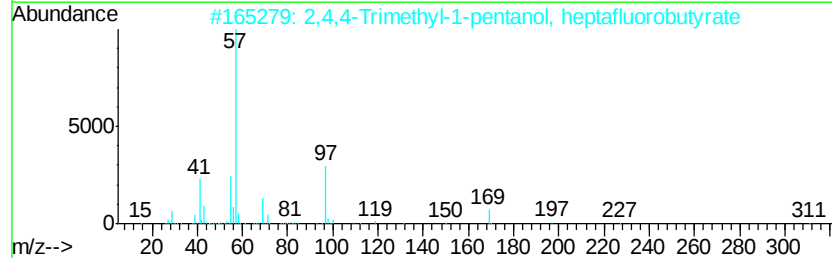
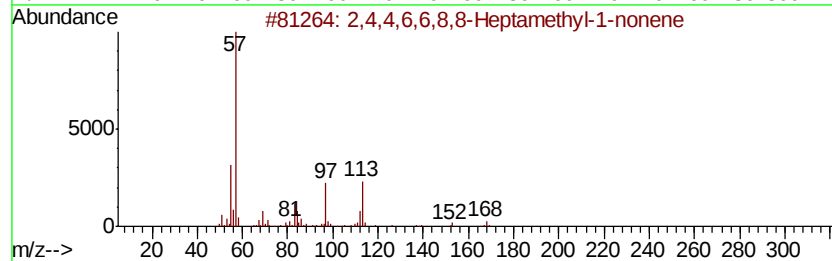
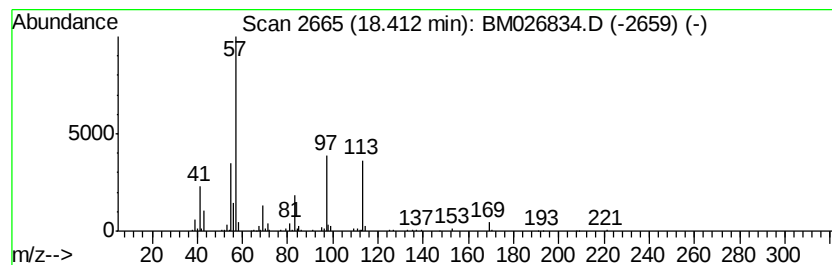
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.41 | 4.41 ng | 218233 | Phenanthrene-d10 | 16.72 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 2,4,4,6,6,8,8-Heptamethyl-1-nonene  | 224 | C16H32     | 015796-04-0  | 50   |
| 2    |    |   | 2,4,4-Trimethyl-1-pentanol, hept... | 326 | C12H17F7O2 | 1000365-01-4 | 47   |
| 3    |    |   | 2,4,4-Trimethyl-1-pentanol, pent... | 276 | C11H17F5O2 | 1000365-51-0 | 43   |
| 4    |    |   | 1-Pentanol, 3-methyl-2-propyl-      | 144 | C9H20O     | 054004-40-9  | 42   |
| 5    |    |   | Pentane, 2,2,4-trimethyl-4-nitro-   | 159 | C8H17NO2   | 005342-78-9  | 40   |



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Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
TP-3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM070820.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

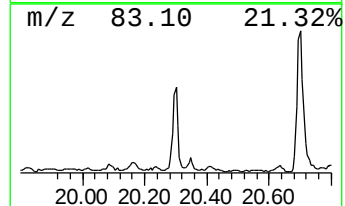
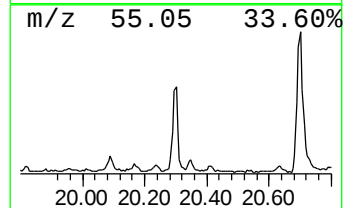
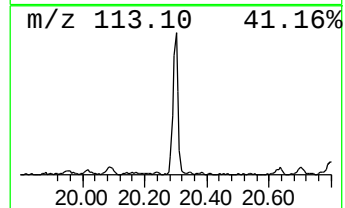
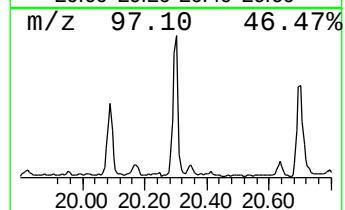
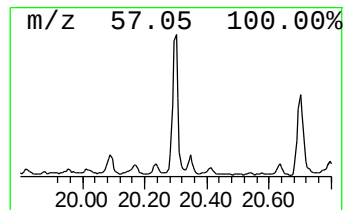
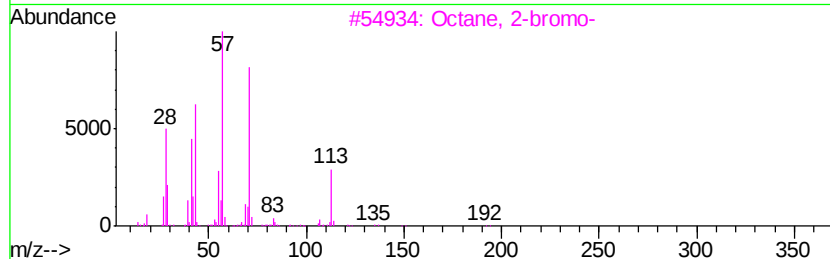
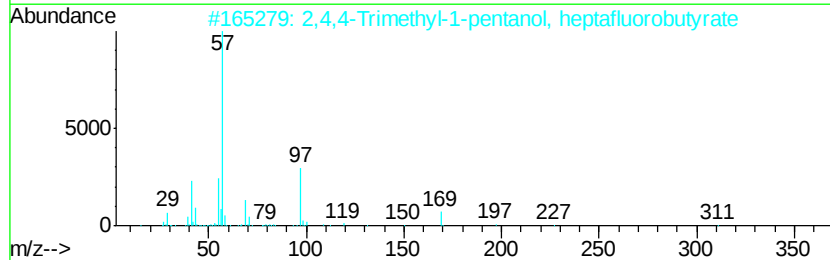
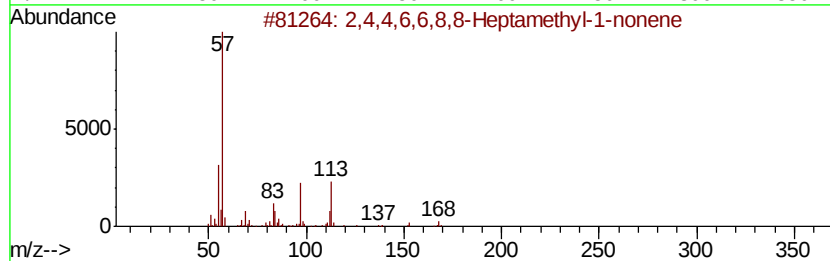
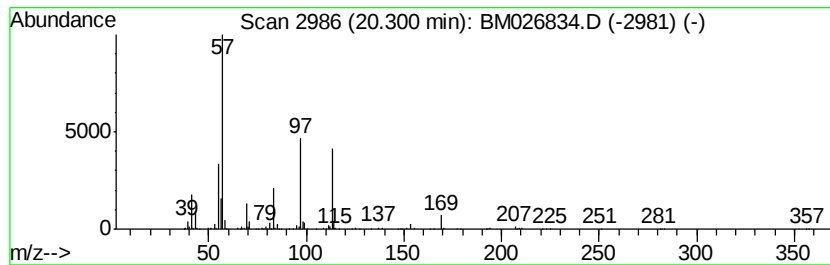
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown20.30 Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.30 | 5.12 ng | 283022 | Chrysene-d12     | 20.95 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | 2,4,4,6,6,8,8-Heptamethyl-1-nonene  | 224 | C16H32      | 015796-04-0  | 45   |
| 2    |    | 2,4,4-Trimethyl-1-pentanol, hept... | 326 | C12H17F7O2  | 1000365-01-4 | 38   |
| 3    |    | Octane, 2-bromo-                    | 192 | C8H17Br     | 000557-35-7  | 37   |
| 4    |    | 1-Pentanol, 3-methyl-2-propyl-      | 144 | C9H20O      | 054004-40-9  | 33   |
| 5    |    | 2,2-Dimethyl-3-pentanol, chlorod... | 228 | C9H15ClF2O2 | 1000376-26-4 | 27   |



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ALS Vial : 6 Sample Multiplier: 1

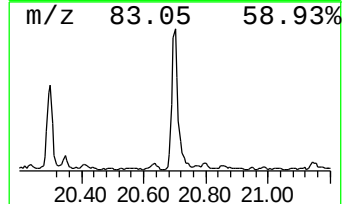
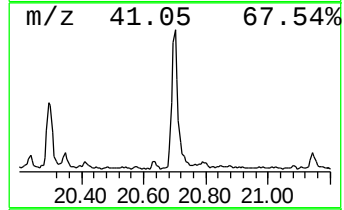
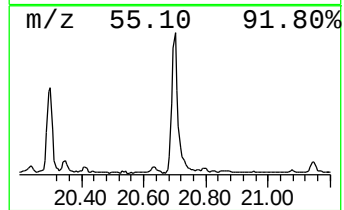
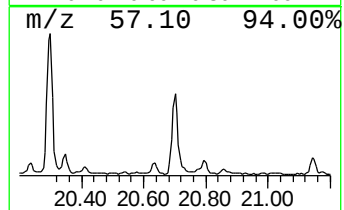
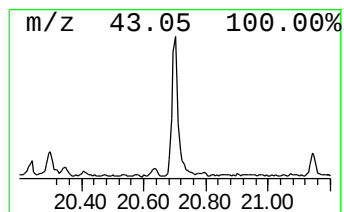
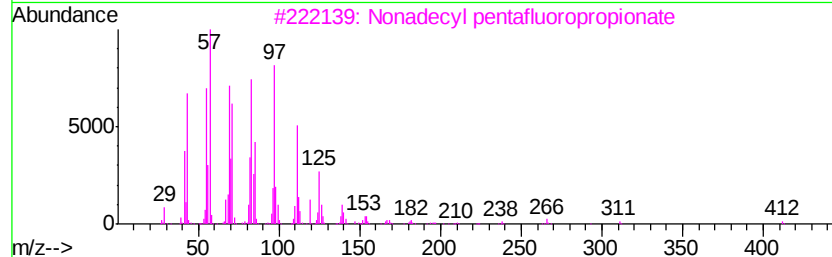
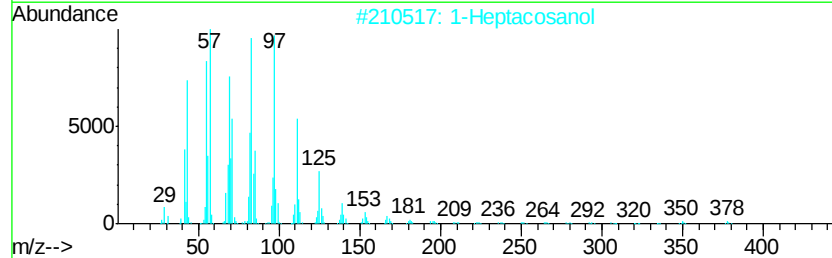
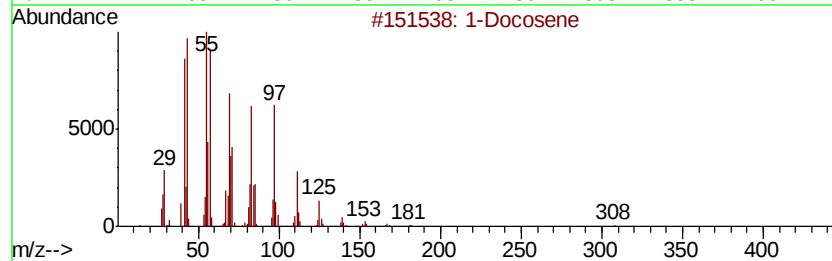
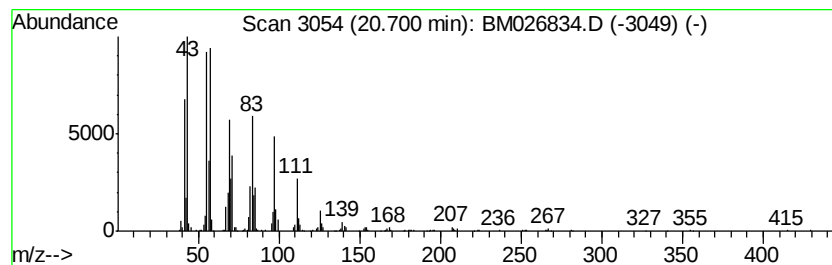
Instrument :  
BNA\_M  
ClientSampleId :  
TP-3-D

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

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Peak Number 4 1-Docosene Concentration Rank 1

| R.T.    | EstConc                             | Area           | Relative to ISTD | R.T.      |
|---------|-------------------------------------|----------------|------------------|-----------|
| 20.70   | 9.73 ng                             | 537740         | Chrysene-d12     | 20.95     |
| Hit# of | 5                                   | Tentative ID   | MW MolForm       | CAS# Qual |
| 1       | 1-Docosene                          | 308 C22H44     | 001599-67-3      | 94        |
| 2       | 1-Heptacosanol                      | 396 C27H56O    | 002004-39-9      | 91        |
| 3       | Nonadecyl pentafluoropropionate     | 430 C22H39F5O2 | 1000351-88-8     | 91        |
| 4       | Heptafluorobutyric acid, hexadec... | 438 C20H33F7O2 | 006385-15-5      | 91        |
| 5       | Trifluoroacetic acid, pentadecyl... | 324 C17H31F3O2 | 959010-23-2      | 91        |



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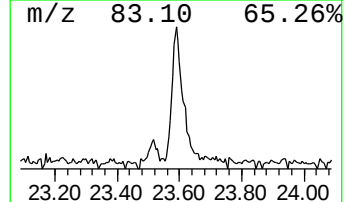
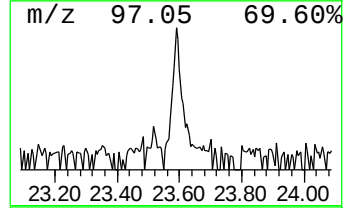
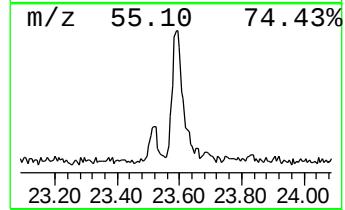
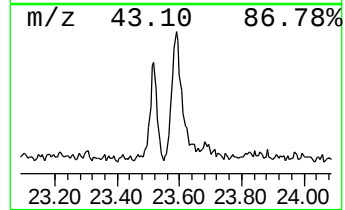
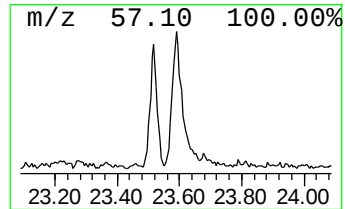
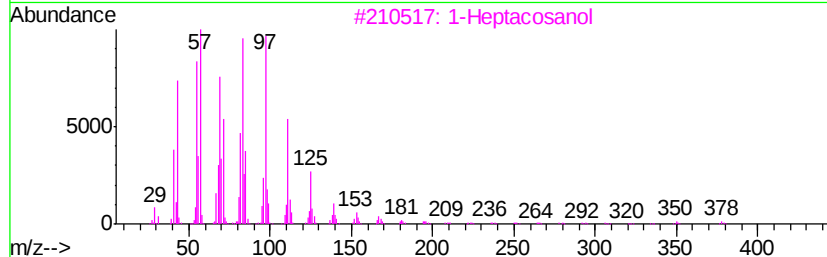
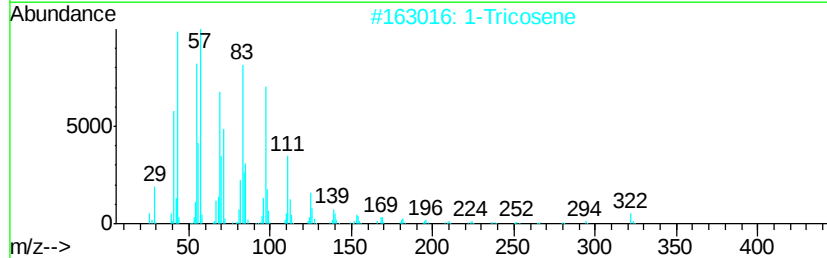
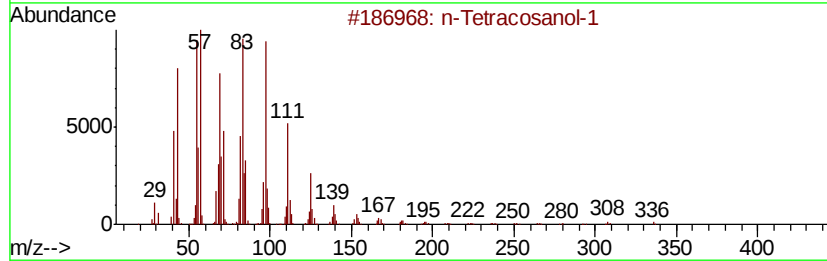
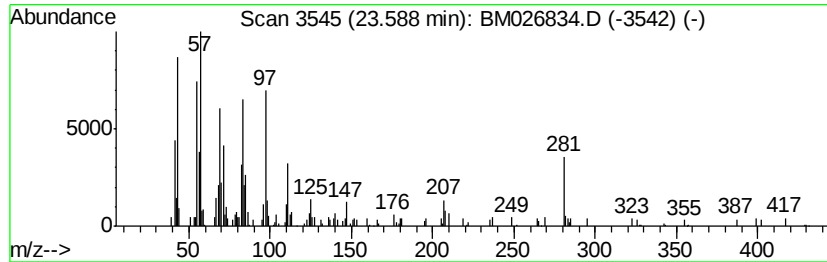
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 n-Tetracosanol-1 Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 23.59 | 2.29 ng | 111760 | Perylene-d12     | 23.02 |

| Hit# | of | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|----|------------------|-----|---------|-------------|------|
| 1    | 5  | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 87   |
| 2    |    | 1-Tricosene      | 322 | C23H46  | 018835-32-0 | 83   |
| 3    |    | 1-Heptacosanol   | 396 | C27H56O | 002004-39-9 | 80   |
| 4    |    | 3-Eicosene, (E)- | 280 | C20H40  | 074685-33-9 | 80   |
| 5    |    | Cyclooctacosane  | 392 | C28H56  | 000297-24-5 | 80   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_M\DATA\BM072220\  
Data File : BM026834.D  
Acq On : 22 Jul 2020 16:12  
Operator : JU/CG  
Sample : L3370-07  
Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
TP-3-D

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM070820.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 |
| n-Hexadecanoic acid  | 17.67 | 3.5     | ng    | 171214   | 4                     | 16.72 | 989510  | 20.0 |
| 2,4,4,6,6,8,8-Hep... | 18.41 | 4.4     | ng    | 218233   | 4                     | 16.72 | 989510  | 20.0 |
| unknown20.30         | 20.30 | 5.1     | ng    | 283022   | 5                     | 20.95 | 1105090 | 20.0 |
| 1-Docosene           | 20.70 | 9.7     | ng    | 537740   | 5                     | 20.95 | 1105090 | 20.0 |
| n-Tetracosanol-1     | 23.59 | 2.3     | ng    | 111760   | 6                     | 23.02 | 977084  | 20.0 |