

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF101718\  
 Data File : BF109933.D  
 Acq On : 17 Oct 2018 21:15  
 Operator : JU/SJ  
 Sample : J5539-02  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-8-3-5FT

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-BF101518.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         | 2.334       | 37            | 42          | 59           | rVB      | 644251         | 895632        | 17.90%          | 1.916%        |
| 2         | 5.216       | 524           | 532         | 544          | rBV      | 163043         | 215245        | 4.30%           | 0.460%        |
| 3         | 5.598       | 592           | 597         | 600          | rBV      | 4851353        | 4588107       | 91.70%          | 9.815%        |
| 4         | 6.592       | 760           | 766         | 771          | rBV      | 4328942        | 4904690       | 98.02%          | 10.492%       |
| 5         | 6.745       | 787           | 792         | 795          | rBV      | 5161361        | 4758578       | 95.10%          | 10.179%       |
| 6         | 6.975       | 828           | 831         | 835          | rVB      | 1731627        | 1411527       | 28.21%          | 3.019%        |
| 7         | 7.133       | 854           | 858         | 861          | rBV      | 4538249        | 3742517       | 74.80%          | 8.006%        |
| 8         | 7.539       | 921           | 927         | 930          | rBV      | 3202513        | 2948551       | 58.93%          | 6.307%        |
| 9         | 8.257       | 1045          | 1049        | 1053         | rBV      | 2008590        | 1763691       | 35.25%          | 3.773%        |
| 10        | 9.333       | 1227          | 1232        | 1235         | rBV      | 5898351        | 5003577       | 100.00%         | 10.703%       |
| 11        | 9.722       | 1295          | 1298        | 1301         | rBV      | 721285         | 530817        | 10.61%          | 1.135%        |
| 12        | 10.016      | 1345          | 1348        | 1352         | rBV      | 1850215        | 1725297       | 34.48%          | 3.691%        |
| 13        | 10.333      | 1397          | 1402        | 1411         | rBV      | 90789          | 178187        | 3.56%           | 0.381%        |
| 14        | 10.804      | 1478          | 1482        | 1486         | rBV      | 2489860        | 2296723       | 45.90%          | 4.913%        |
| 15        | 11.510      | 1598          | 1602        | 1605         | rBV      | 1605229        | 1355503       | 27.09%          | 2.900%        |
| 16        | 12.015      | 1685          | 1688        | 1694         | rBV      | 192267         | 206300        | 4.12%           | 0.441%        |
| 17        | 12.804      | 1819          | 1822        | 1827         | rBV5     | 59124          | 81350         | 1.63%           | 0.174%        |
| 18        | 13.092      | 1867          | 1871        | 1874         | rBV      | 3855214        | 3236072       | 64.68%          | 6.922%        |
| 19        | 13.310      | 1906          | 1908        | 1913         | rVB      | 92437          | 84134         | 1.68%           | 0.180%        |
| 20        | 13.651      | 1964          | 1966        | 1968         | rVB      | 99377          | 76501         | 1.53%           | 0.164%        |
| 21        | 13.974      | 2018          | 2021        | 2031         | rBV2     | 454881         | 573840        | 11.47%          | 1.228%        |
| 22        | 14.151      | 2048          | 2051        | 2054         | rBV      | 1423188        | 1245059       | 24.88%          | 2.663%        |
| 23        | 14.298      | 2073          | 2076        | 2079         | rVB      | 240554         | 203170        | 4.06%           | 0.435%        |
| 24        | 14.604      | 2125          | 2128        | 2133         | rVB2     | 460887         | 477203        | 9.54%           | 1.021%        |
| 25        | 14.927      | 2179          | 2183        | 2186         | rBV      | 462903         | 459342        | 9.18%           | 0.983%        |
| 26        | 15.280      | 2239          | 2243        | 2252         | rVB      | 601470         | 792942        | 15.85%          | 1.696%        |
| 27        | 15.680      | 2306          | 2311        | 2318         | rVB2     | 1328968        | 1895952       | 37.89%          | 4.056%        |
| 28        | 16.151      | 2386          | 2391        | 2397         | rVB      | 412459         | 636878        | 12.73%          | 1.362%        |
| 29        | 16.692      | 2478          | 2483        | 2493         | rVB2     | 234200         | 460563        | 9.20%           | 0.985%        |

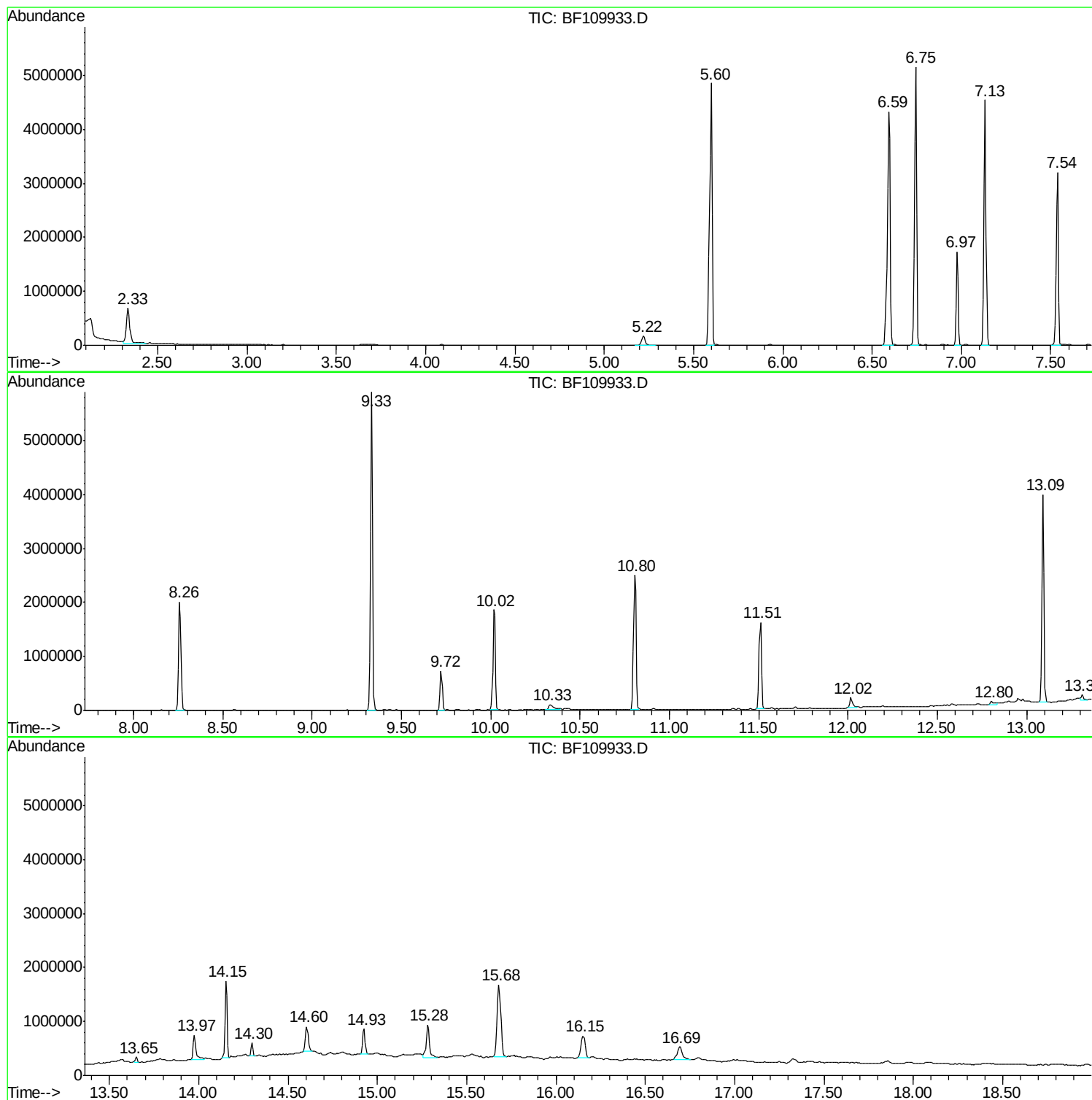
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BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101518.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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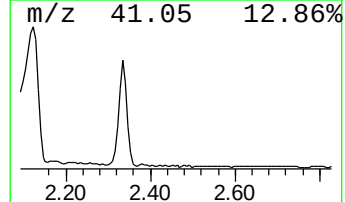
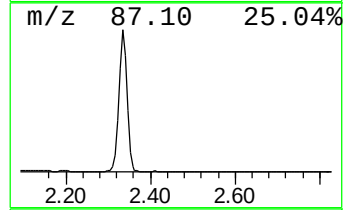
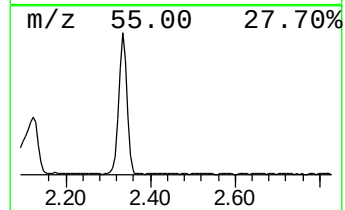
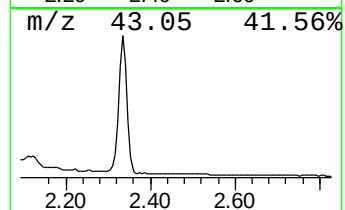
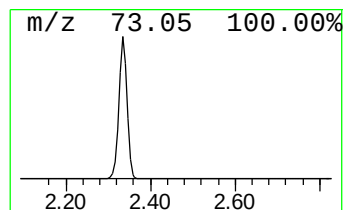
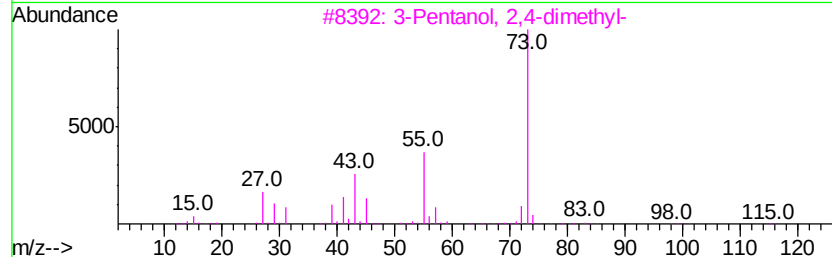
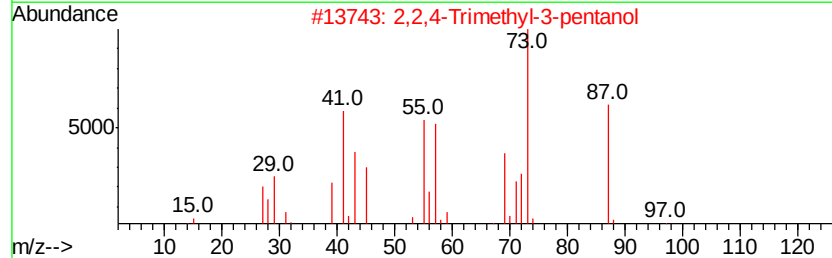
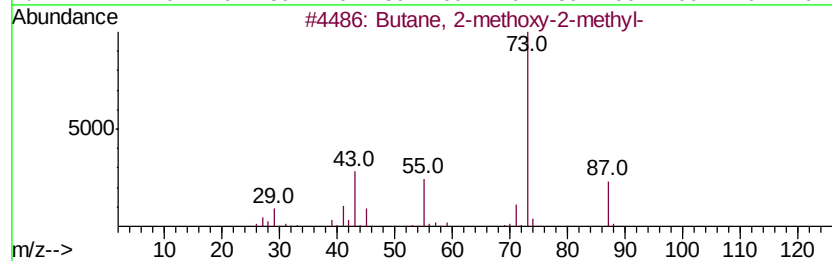
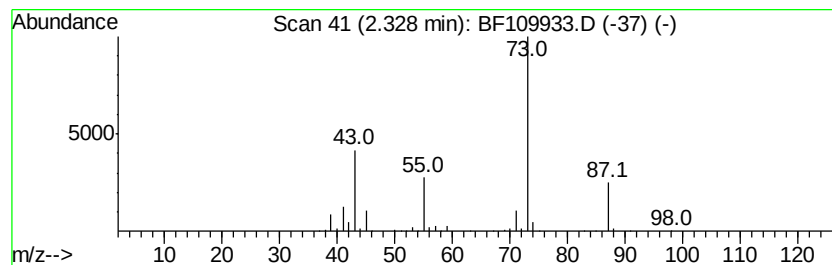
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 2.33 | 12.69 ng | 895632 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 37   |
| 4    |    | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 25   |
| 5    |    | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 12   |



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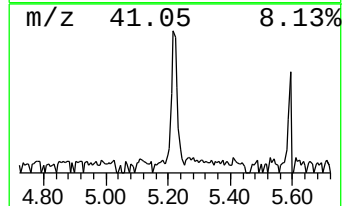
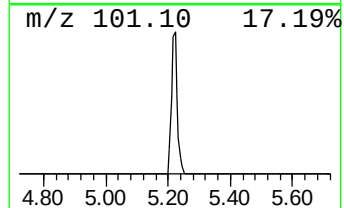
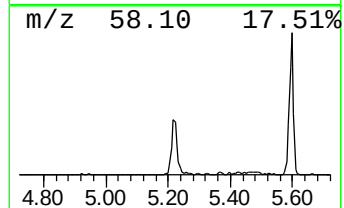
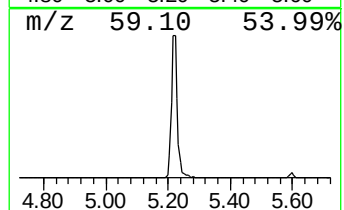
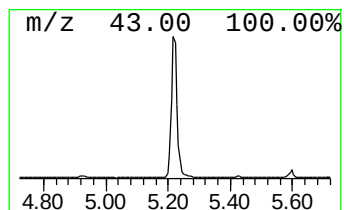
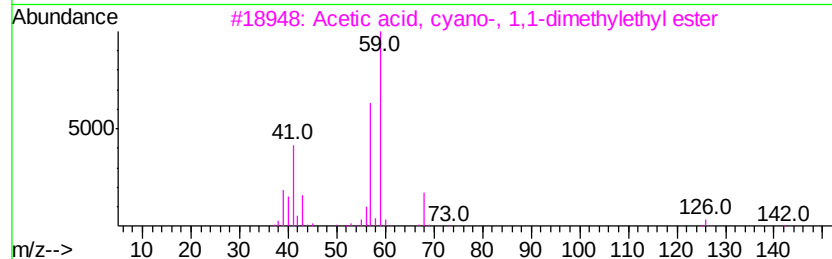
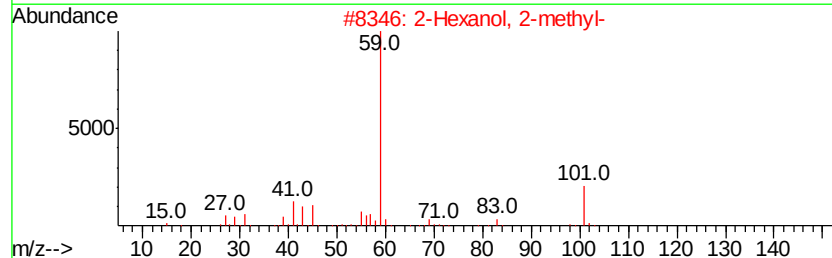
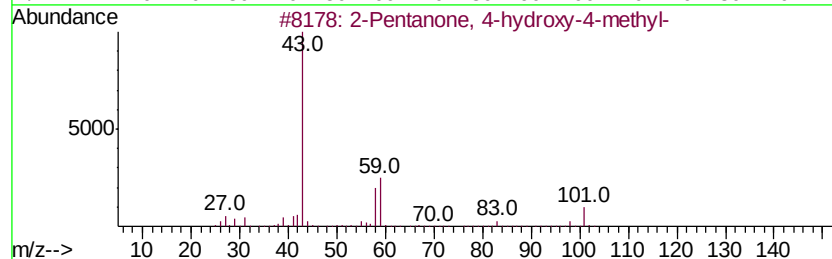
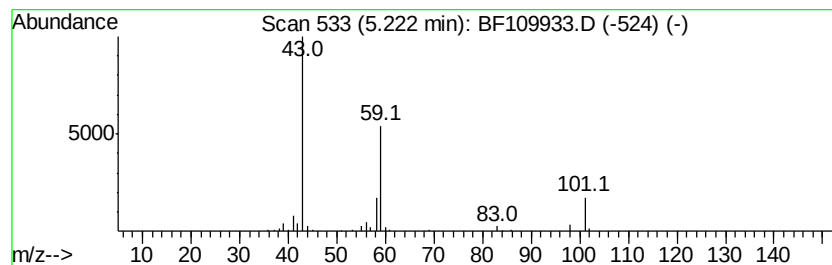
Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.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-Pentanone, 4-hydroxy-4-me... Concentration Rank 11

| R.T.      | EstConc                              | Area   | Relative to ISTD       | R.T.        |      |
|-----------|--------------------------------------|--------|------------------------|-------------|------|
| 5.22      | 3.05 ng                              | 215245 | 1,4-Dichlorobenzene-d4 | 6.97        |      |
| Hit# of 5 | Tentative ID                         | MW     | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-     | 116    | C6H12O2                | 000123-42-2 | 59   |
| 2         | 2-Hexanol, 2-methyl-                 | 116    | C7H16O                 | 000625-23-0 | 28   |
| 3         | Acetic acid, cyano-, 1,1-dimethyl... | 141    | C7H11NO2               | 001116-98-9 | 25   |
| 4         | 2,3-Butanedione, monooxime           | 101    | C4H7NO2                | 000057-71-6 | 16   |
| 5         | 1-Propen-2-ol, acetate               | 100    | C5H8O2                 | 000108-22-5 | 10   |



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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

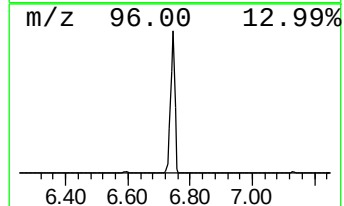
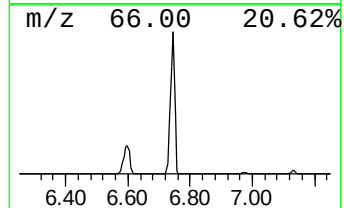
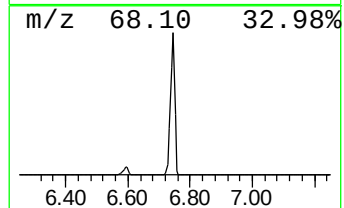
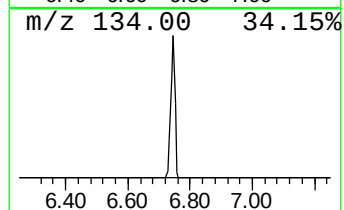
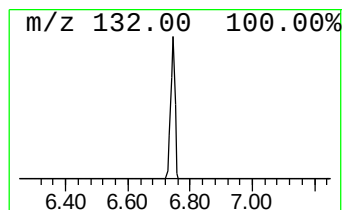
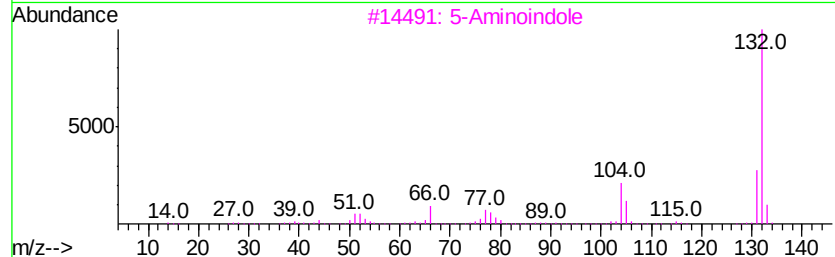
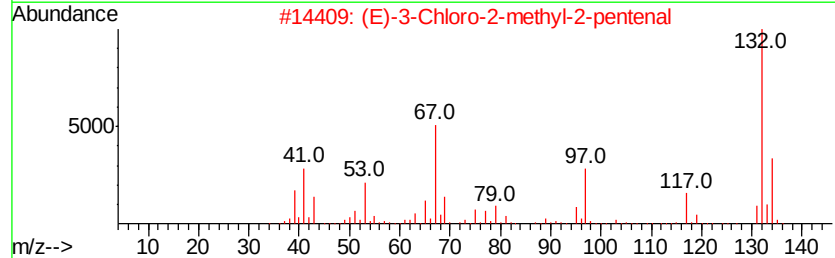
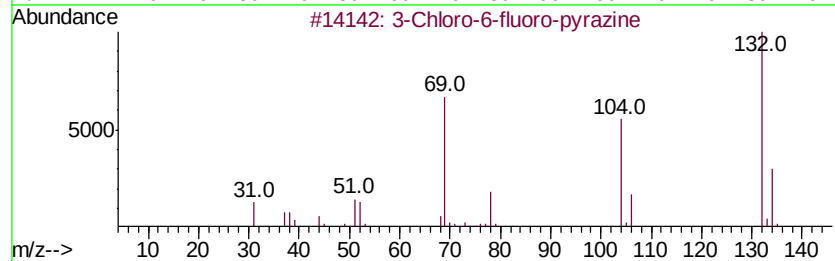
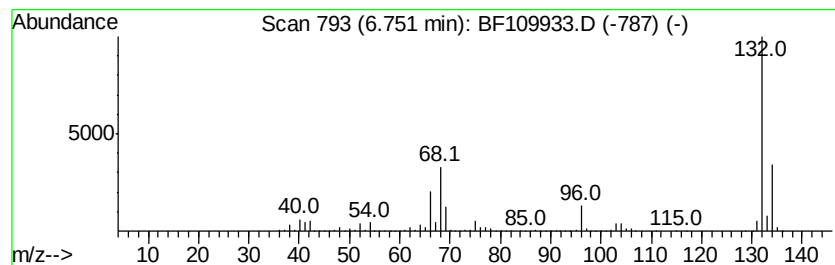
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 unknown6.75 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.75 | 67.42 ng | 4758580 | 1,4-Dichlorobenzene-d4 | 6.97 |

| 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  | 17   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-59-9  | 9    |



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BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

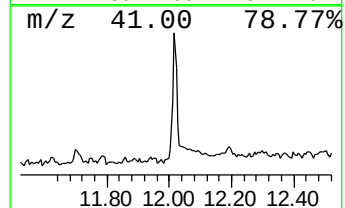
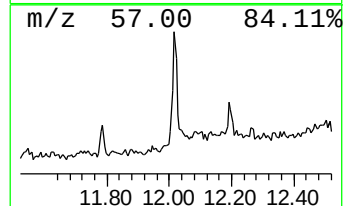
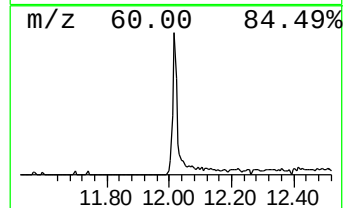
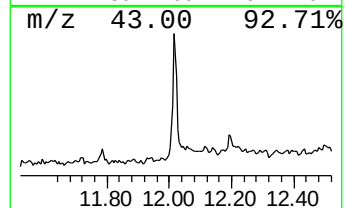
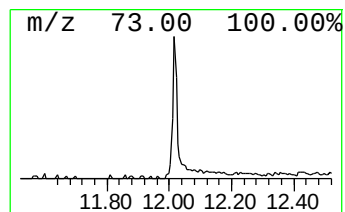
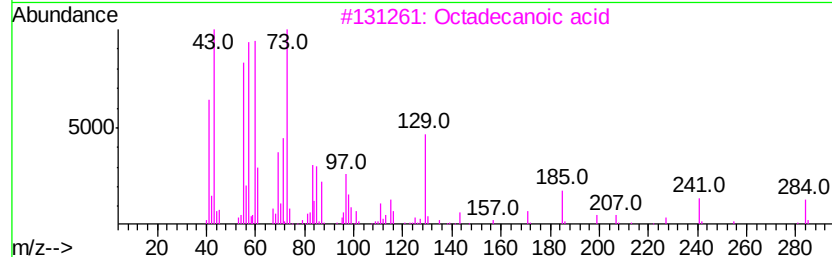
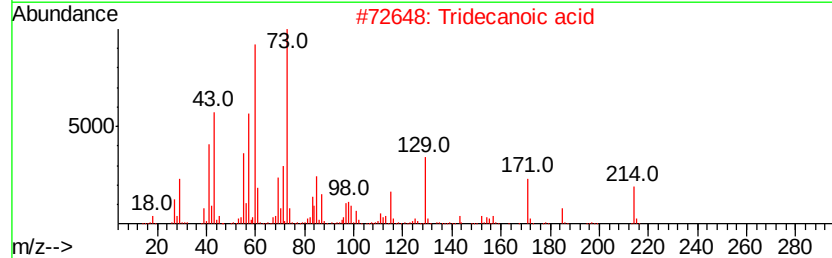
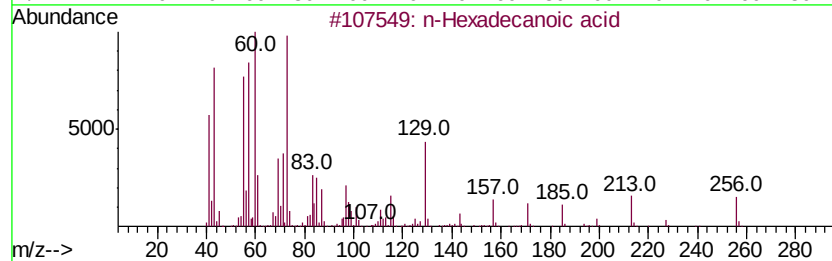
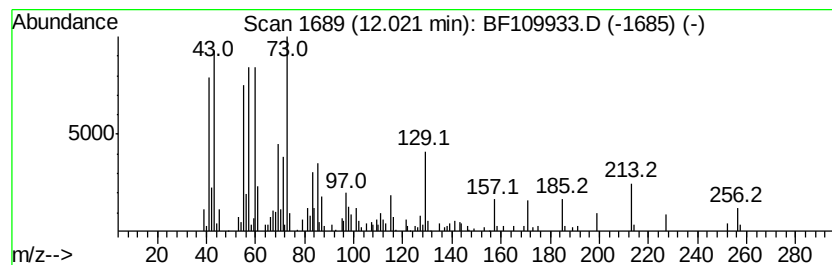
TIC Library : C:\DATABASE\NIST11.L  
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Peak Number 6 n-Hexadecanoic acid Concentration Rank 12

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.02 | 3.04 ng | 206300 | Phenanthrene-d10 | 11.51 |

| Hit# of 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|-----------|---------------------|-----|----------|-------------|------|
| 1         | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2         | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 3         | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 90   |
| 4         | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 5         | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 72   |



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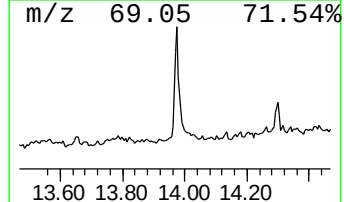
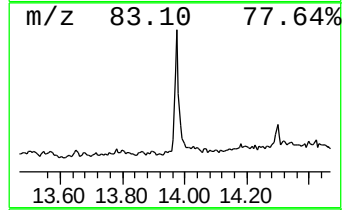
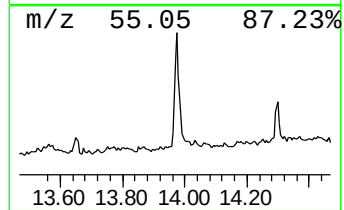
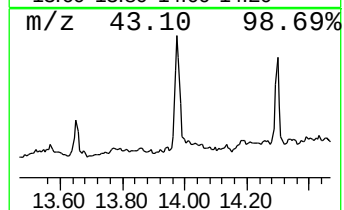
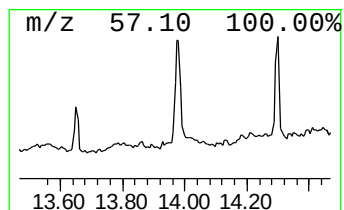
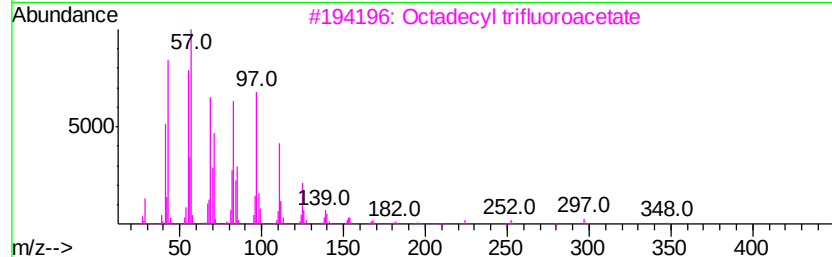
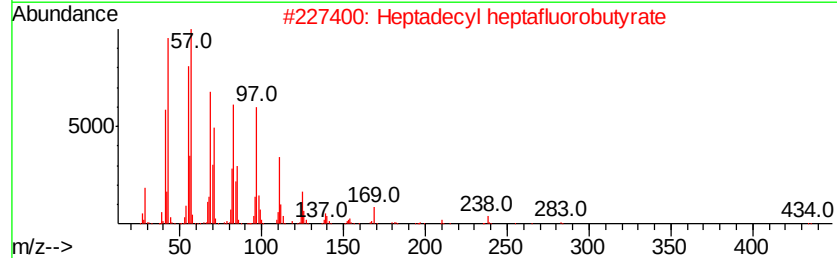
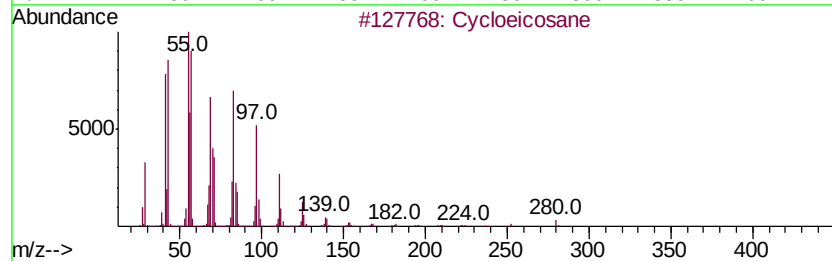
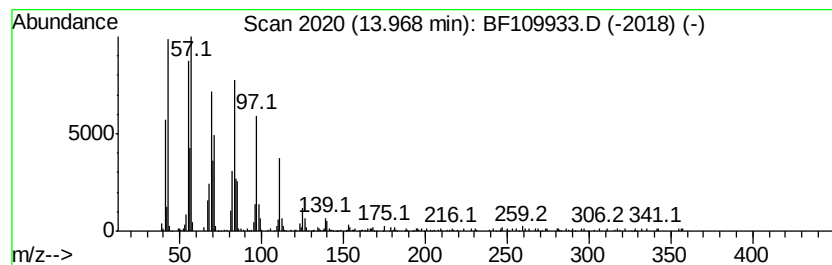
Instrument :  
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Cycloeicosane Concentration Rank 4

| R.T.    | EstConc | Area                           | Relative to ISTD | R.T.            |
|---------|---------|--------------------------------|------------------|-----------------|
| 13.97   | 9.22 ng | 573840                         | Chrysene-d12     | 14.15           |
| Hit# of | 5       | Tentative ID                   | MW MolForm       | CAS# Qual       |
| 1       |         | Cycloeicosane                  | 280 C20H40       | 000296-56-0 98  |
| 2       |         | Heptadecyl heptafluorobutyrate | 452 C21H35F7O2   | 959085-66-6 94  |
| 3       |         | Octadecyl trifluoroacetate     | 366 C20H37F3O2   | 079392-43-1 91  |
| 4       |         | 1-Hexadecanesulfonyl chloride  | 324 C16H33ClO2S  | 038775-38-1 91  |
| 5       |         | Tricosyl trifluoroacetate      | 436 C25H47F3O2   | 1000351-75-1 91 |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\  
Data File : BF109933.D  
Acq On : 17 Oct 2018 21:15  
Operator : JU/SJ  
Sample : J5539-02  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

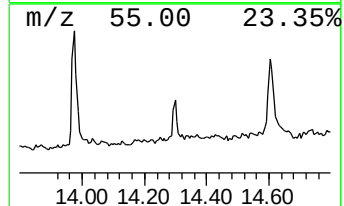
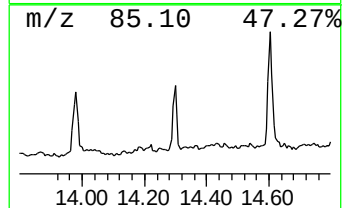
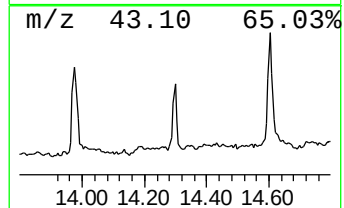
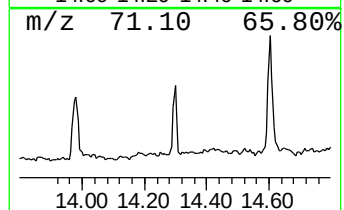
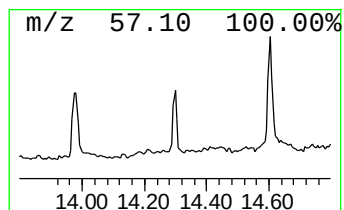
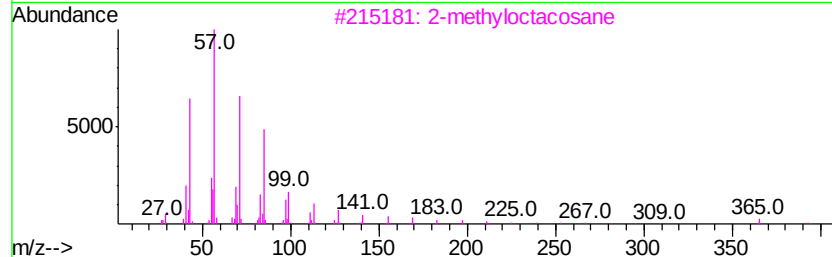
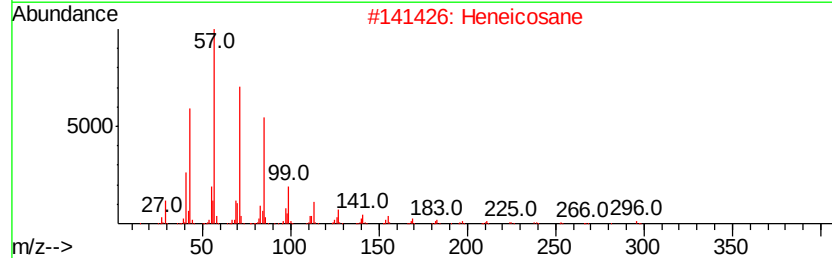
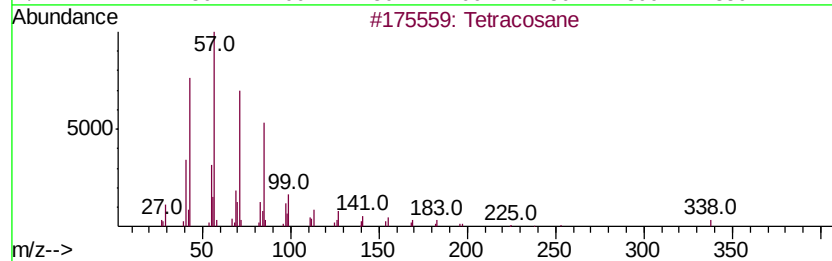
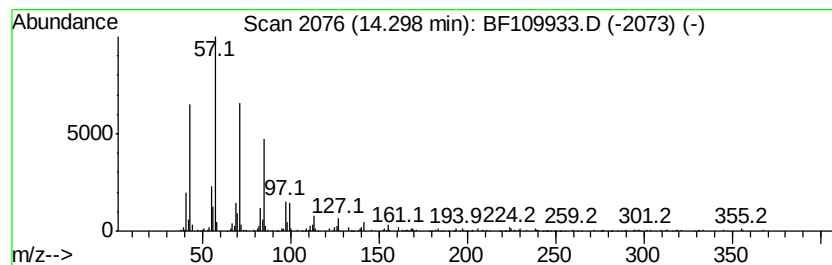
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Tetracosane Concentration Rank 10

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.30 | 3.26 ng | 203170 | Chrysene-d12     | 14.15 |

| Hit# of | 5 | Tentative ID       | MW  | MolForm | CAS#         | Qual |
|---------|---|--------------------|-----|---------|--------------|------|
| 1       |   | Tetracosane        | 338 | C24H50  | 000646-31-1  | 87   |
| 2       |   | Heneicosane        | 296 | C21H44  | 000629-94-7  | 87   |
| 3       |   | 2-methyloctacosane | 408 | C29H60  | 1000376-72-8 | 87   |
| 4       |   | Hexacosane         | 366 | C26H54  | 000630-01-3  | 86   |
| 5       |   | Octadecane         | 254 | C18H38  | 000593-45-3  | 83   |





Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\  
Data File : BF109933.D  
Acq On : 17 Oct 2018 21:15  
Operator : JU/SJ  
Sample : J5539-02  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

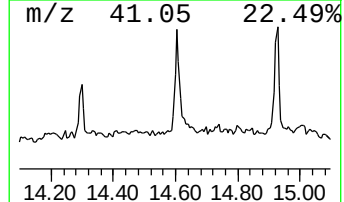
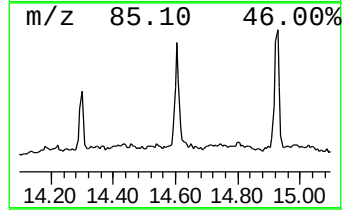
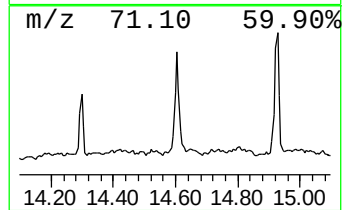
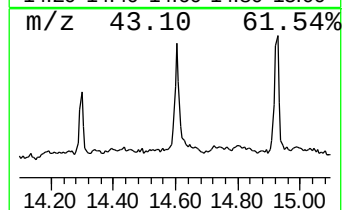
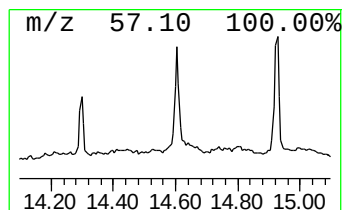
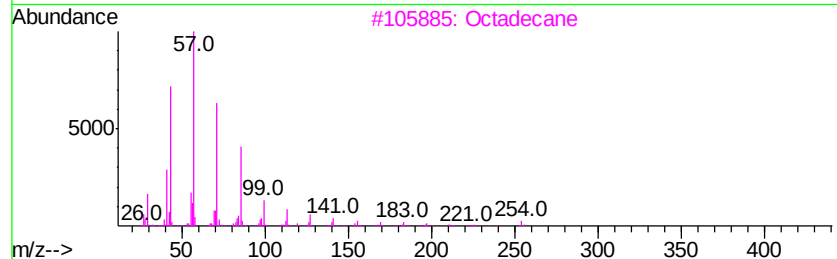
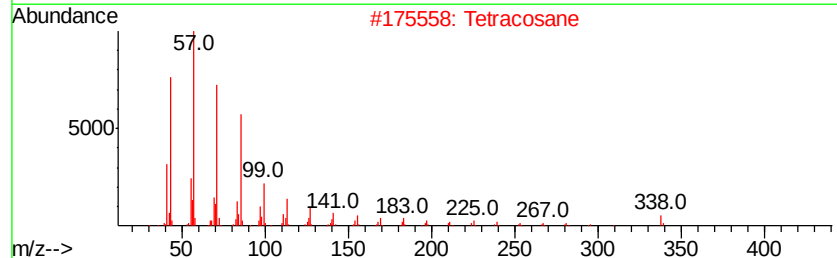
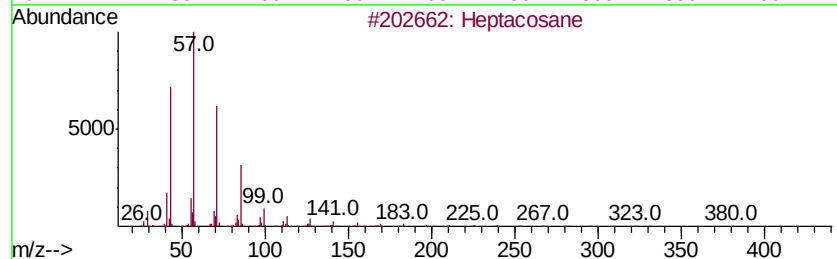
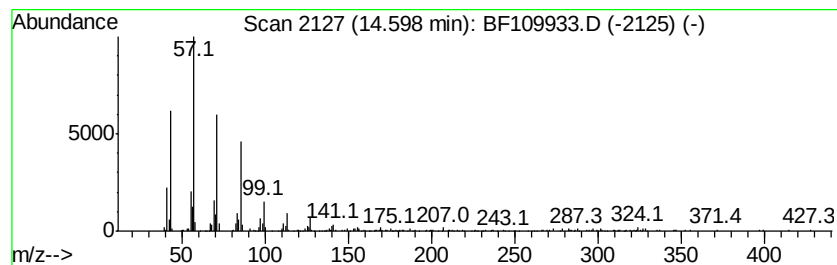
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 Heptacosane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.60 | 7.67 ng | 477203 | Chrysene-d12     | 14.15 |

| Hit# | of | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------------|-----|---------|-------------|------|
| 1    | 5  | Heptacosane           | 380 | C27H56  | 000593-49-7 | 93   |
| 2    |    | Tetracosane           | 338 | C24H50  | 000646-31-1 | 93   |
| 3    |    | Octadecane            | 254 | C18H38  | 000593-45-3 | 91   |
| 4    |    | Decane, 3,8-dimethyl- | 170 | C12H26  | 017312-55-9 | 87   |
| 5    |    | Hexacosane            | 366 | C26H54  | 000630-01-3 | 87   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\  
Data File : BF109933.D  
Acq On : 17 Oct 2018 21:15  
Operator : JU/SJ  
Sample : J5539-02  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

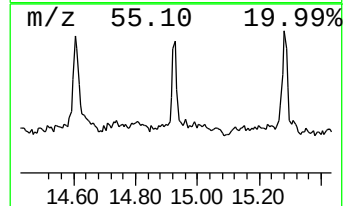
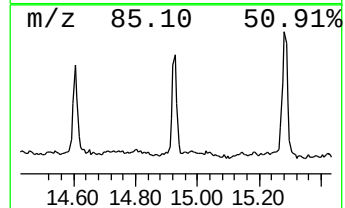
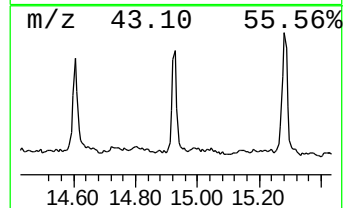
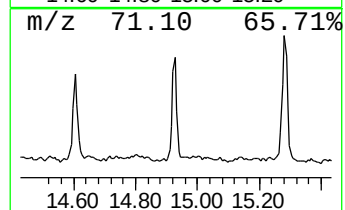
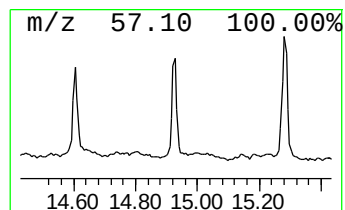
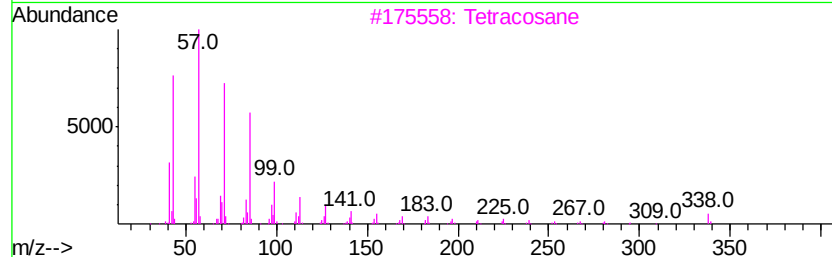
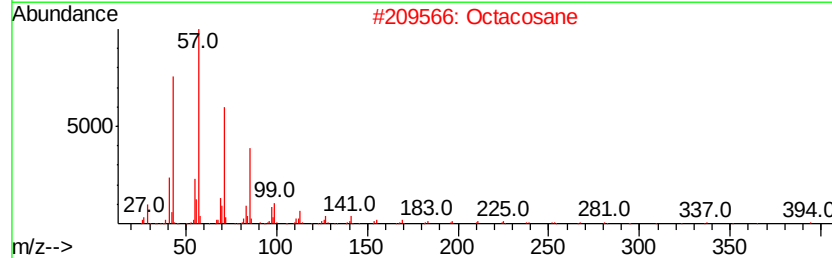
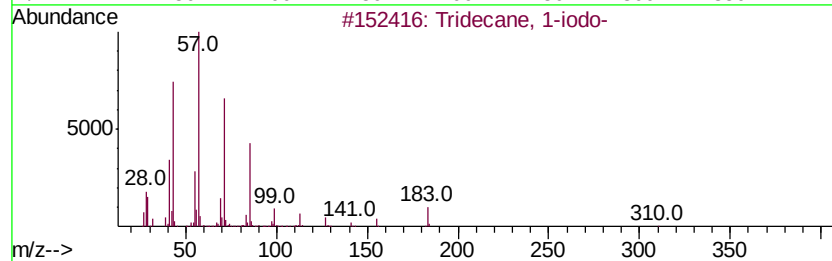
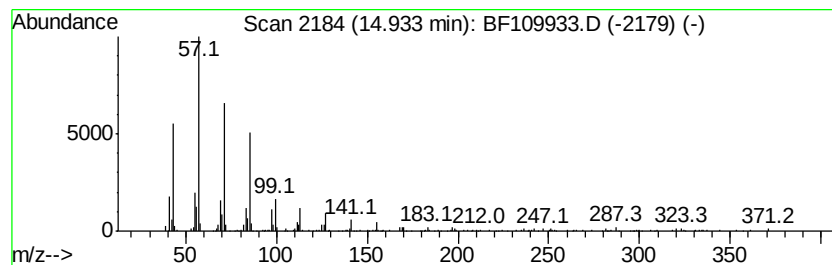
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 10 Tridecane, 1-iodo- Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.93 | 4.85 ng | 459342 | Perylene-d12     | 15.68 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------|-----|---------|-------------|------|
| 1    |    |   | Tridecane, 1-iodo-    | 310 | C13H27I | 035599-77-0 | 93   |
| 2    |    |   | Octacosane            | 394 | C28H58  | 000630-02-4 | 91   |
| 3    |    |   | Tetracosane           | 338 | C24H50  | 000646-31-1 | 91   |
| 4    |    |   | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1 | 91   |
| 5    |    |   | Hexacosane            | 366 | C26H54  | 000630-01-3 | 90   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF101718\  
Data File : BF109933.D  
Acq On : 17 Oct 2018 21:15  
Operator : JU/SJ  
Sample : J5539-02  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

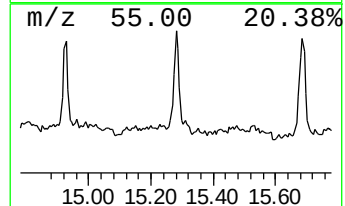
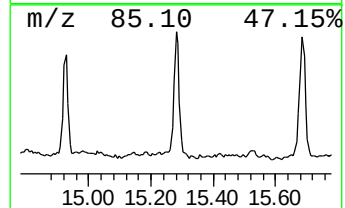
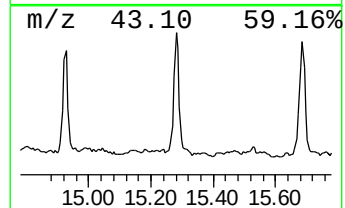
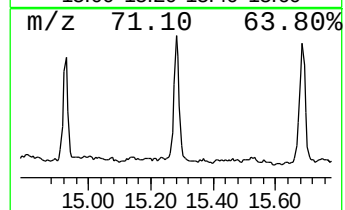
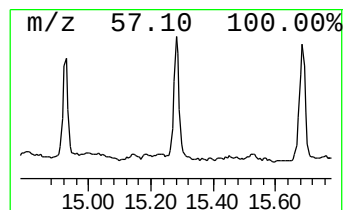
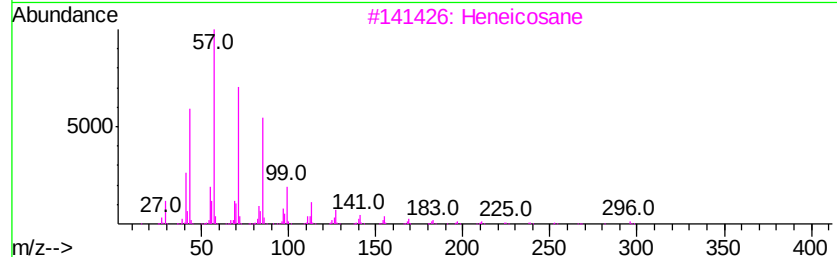
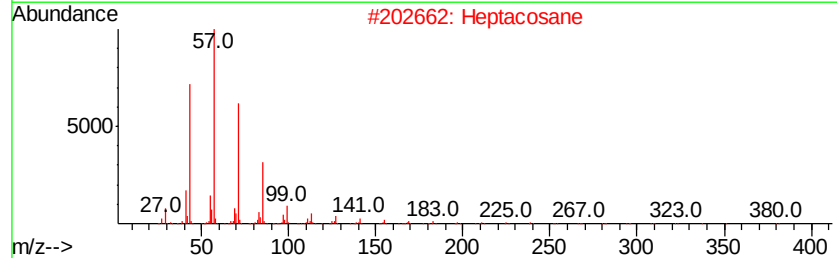
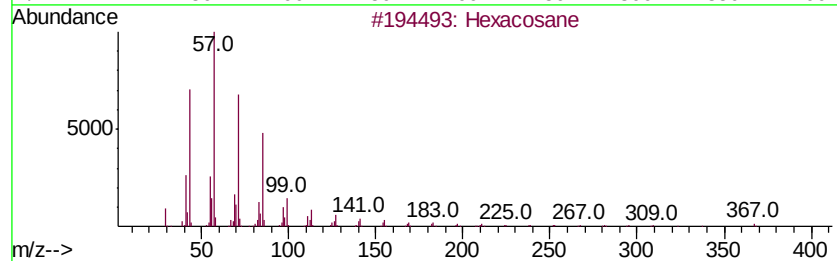
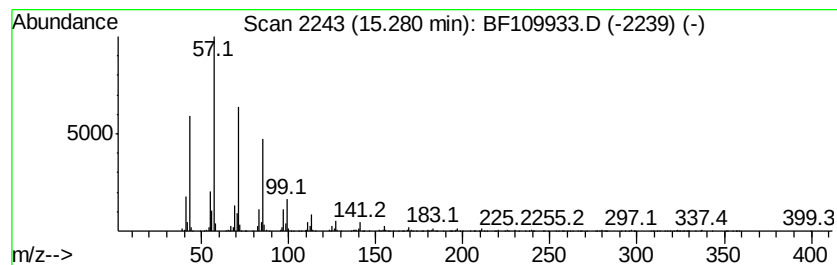
Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF101518.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 11 Hexacosane Concentration Rank 5

| R.T.      | EstConc      | Area   | Relative to ISTD |             | R.T.  |
|-----------|--------------|--------|------------------|-------------|-------|
| 15.28     | 8.36 ng      | 792942 | Perylene-d12     |             | 15.68 |
| Hit# of 5 | Tentative ID | MW     | MolForm          | CAS#        | Qual  |
| 1         | Hexacosane   | 366    | C26H54           | 000630-01-3 | 91    |
| 2         | Heptacosane  | 380    | C27H56           | 000593-49-7 | 91    |
| 3         | Heneicosane  | 296    | C21H44           | 000629-94-7 | 90    |
| 4         | Tetracosane  | 338    | C24H50           | 000646-31-1 | 87    |
| 5         | Tricosane    | 324    | C23H48           | 000638-67-5 | 87    |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF101718\  
Data File : BF109933.D  
Acq On : 17 Oct 2018 21:15  
Operator : JU/SJ  
Sample : J5539-02  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-8-3-5FT

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF101518.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 |
| Butane, 2-methoxy... | 2.33  | 12.7    | ng    | 895632   | 1                     | 6.97  | 1411530 | 20.0 |
| 2-Pentanone, 4-hy... | 5.22  | 3.0     | ng    | 215245   | 1                     | 6.97  | 1411530 | 20.0 |
| unknown6.75          | 6.75  | 67.4    | ng    | 4758580  | 1                     | 6.97  | 1411530 | 20.0 |
| n-Hexadecanoic acid  | 12.02 | 3.0     | ng    | 206300   | 4                     | 11.51 | 1355500 | 20.0 |
| Cycloeicosane        | 13.97 | 9.2     | ng    | 573840   | 5                     | 14.15 | 1245060 | 20.0 |
| Tetracosane          | 14.30 | 3.3     | ng    | 203170   | 5                     | 14.15 | 1245060 | 20.0 |
| Heptacosane          | 14.60 | 7.7     | ng    | 477203   | 5                     | 14.15 | 1245060 | 20.0 |
| Tridecane, 1-iodo-   | 14.93 | 4.8     | ng    | 459342   | 6                     | 15.68 | 1895950 | 20.0 |
| Hexacosane           | 15.28 | 8.4     | ng    | 792942   | 6                     | 15.68 | 1895950 | 20.0 |