

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030917\  
 Data File : BF093500.D  
 Acq On : 10 Mar 2017 2:42  
 Operator : SJ/MA  
 Sample : I2188-02  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RU-BUBBLE-01

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:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.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         | 1.955       | 3             | 6           | 10           | rBV      | 63190          | 105077        | 1.93%           | 0.234%        |
| 2         | 4.241       | 204           | 206         | 211          | rBV      | 35772          | 76732         | 1.41%           | 0.171%        |
| 3         | 4.904       | 262           | 264         | 282          | rBV      | 638461         | 1135087       | 20.85%          | 2.523%        |
| 4         | 5.350       | 301           | 303         | 319          | rBV      | 4287249        | 4974418       | 91.36%          | 11.058%       |
| 5         | 5.750       | 334           | 338         | 343          | rVB2     | 39676          | 57201         | 1.05%           | 0.127%        |
| 6         | 6.413       | 393           | 396         | 403          | rBV      | 3451992        | 5444570       | 100.00%         | 12.103%       |
| 7         | 6.527       | 403           | 406         | 408          | rVV      | 3477053        | 4768364       | 87.58%          | 10.600%       |
| 8         | 6.744       | 423           | 425         | 428          | rBV      | 1099025        | 1164475       | 21.39%          | 2.589%        |
| 9         | 6.904       | 436           | 439         | 441          | rBV      | 3776542        | 3656907       | 67.17%          | 8.129%        |
| 10        | 7.327       | 473           | 476         | 478          | rBV      | 2660087        | 3328237       | 61.13%          | 7.399%        |
| 11        | 8.036       | 535           | 538         | 540          | rBV      | 1689138        | 1536522       | 28.22%          | 3.416%        |
| 12        | 9.110       | 629           | 632         | 634          | rBV      | 4946594        | 4558423       | 83.72%          | 10.133%       |
| 13        | 9.510       | 664           | 667         | 669          | rBV      | 1094799        | 953481        | 17.51%          | 2.120%        |
| 14        | 9.785       | 689           | 691         | 693          | rBV      | 1826103        | 1632756       | 29.99%          | 3.630%        |
| 15        | 10.208      | 727           | 728         | 730          | rVB      | 79710          | 91316         | 1.68%           | 0.203%        |
| 16        | 10.573      | 758           | 760         | 763          | rBV2     | 2089549        | 2384586       | 43.80%          | 5.301%        |
| 17        | 10.699      | 768           | 771         | 774          | rBV2     | 354084         | 488343        | 8.97%           | 1.086%        |
| 18        | 10.756      | 774           | 776         | 777          | rVV      | 86180          | 72316         | 1.33%           | 0.161%        |
| 19        | 10.791      | 777           | 779         | 780          | rVV2     | 62994          | 80678         | 1.48%           | 0.179%        |
| 20        | 10.825      | 780           | 782         | 785          | rVB3     | 63589          | 103159        | 1.89%           | 0.229%        |
| 21        | 10.905      | 785           | 789         | 790          | rBV3     | 40237          | 82483         | 1.51%           | 0.183%        |
| 22        | 10.939      | 790           | 792         | 793          | rVV      | 74879          | 93266         | 1.71%           | 0.207%        |
| 23        | 10.973      | 793           | 795         | 797          | rVV      | 86040          | 96284         | 1.77%           | 0.214%        |
| 24        | 11.008      | 797           | 798         | 801          | rVB2     | 48454          | 56448         | 1.04%           | 0.125%        |
| 25        | 11.133      | 806           | 809         | 810          | rBV      | 134686         | 119721        | 2.20%           | 0.266%        |
| 26        | 11.271      | 819           | 821         | 823          | rBV      | 1637517        | 1512525       | 27.78%          | 3.362%        |
| 27        | 11.328      | 825           | 826         | 831          | rVB      | 57965          | 58478         | 1.07%           | 0.130%        |
| 28        | 11.556      | 844           | 846         | 848          | rVB      | 109050         | 87330         | 1.60%           | 0.194%        |
| 29        | 12.482      | 926           | 927         | 932          | rVB      | 56001          | 68260         | 1.25%           | 0.152%        |
| 30        | 12.711      | 945           | 947         | 949          | rBV      | 50928          | 64178         | 1.18%           | 0.143%        |
| 31        | 12.848      | 957           | 959         | 962          | rBV      | 3031030        | 3226293       | 59.26%          | 7.172%        |
| 32        | 13.751      | 1035          | 1038        | 1043         | rBV      | 176170         | 283164        | 5.20%           | 0.629%        |
| 33        | 13.877      | 1047          | 1049        | 1050         | rBV      | 129602         | 125046        | 2.30%           | 0.278%        |
| 34        | 13.911      | 1050          | 1052        | 1054         | rVV      | 1001327        | 1011214       | 18.57%          | 2.248%        |

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ClientSampleId :  
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Integration Parameters: rteint.p  
Integrator: RTE  
Smoothing : ON Filtering: 5  
Sampling : 1 Min Area: 3 % of largest Peak  
Start Thrs: 0.2 Max Peaks: 100  
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |         |        |        |
|----|--------|------|------|------|------|--------|---------|--------|--------|
| 35 | 14.368 | 1089 | 1092 | 1097 | rBV3 | 39091  | 135835  | 2.49%  | 0.302% |
| 36 | 14.962 | 1142 | 1144 | 1146 | rVB  | 58841  | 73724   | 1.35%  | 0.164% |
| 37 | 15.317 | 1172 | 1175 | 1181 | rVB  | 817808 | 1032233 | 18.96% | 2.295% |
| 38 | 15.694 | 1206 | 1208 | 1211 | rBV  | 43675  | 65278   | 1.20%  | 0.145% |
| 39 | 18.323 | 1435 | 1438 | 1445 | rVB3 | 59809  | 179868  | 3.30%  | 0.400% |

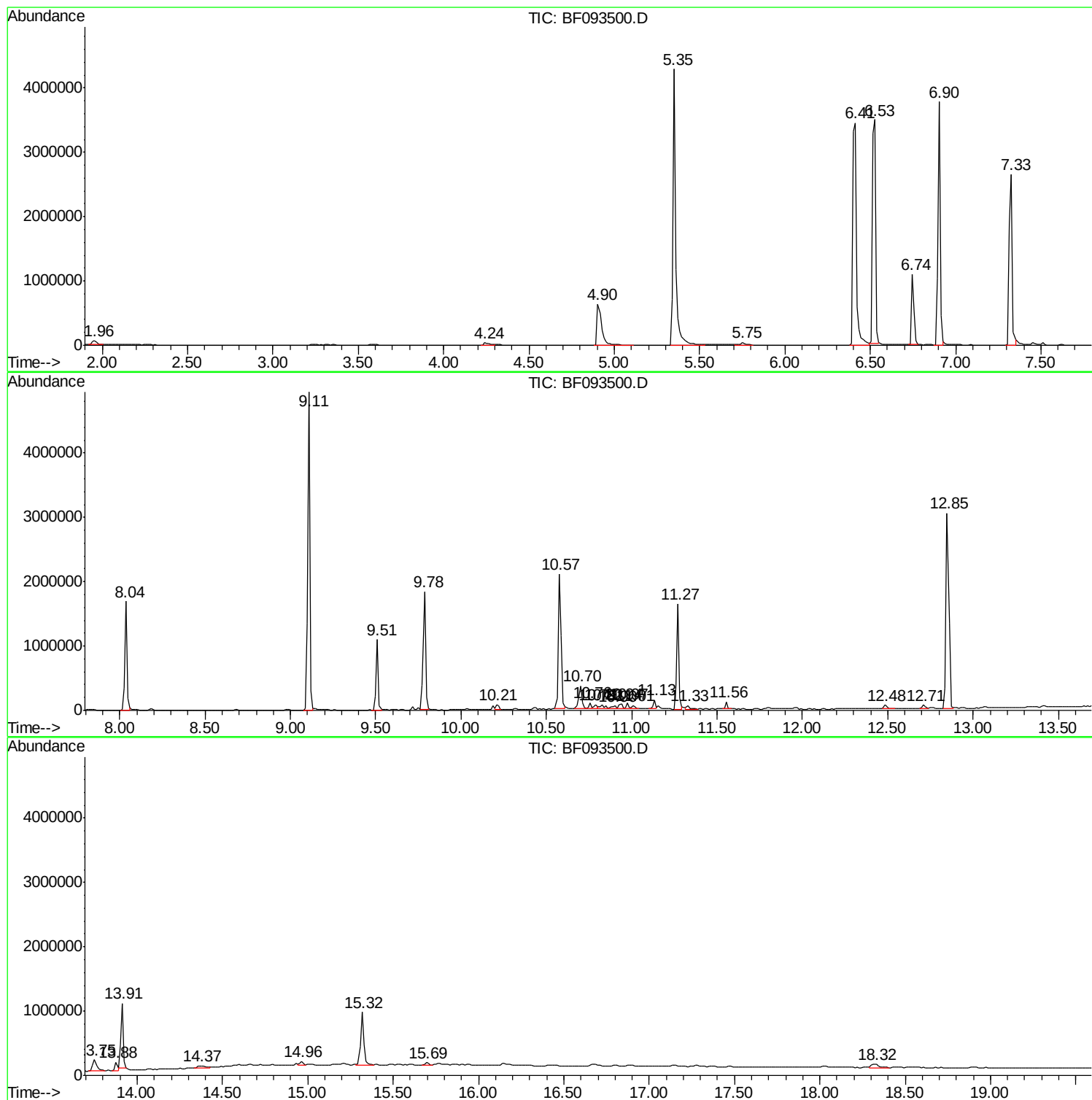
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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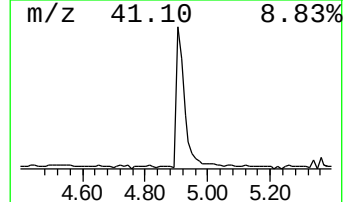
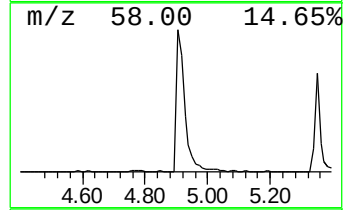
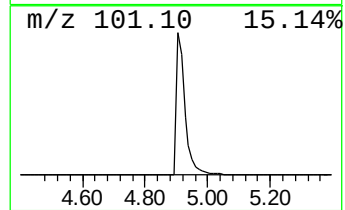
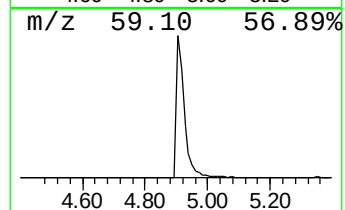
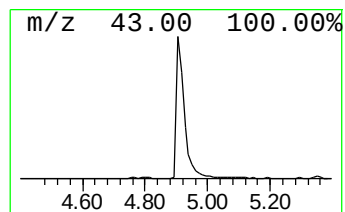
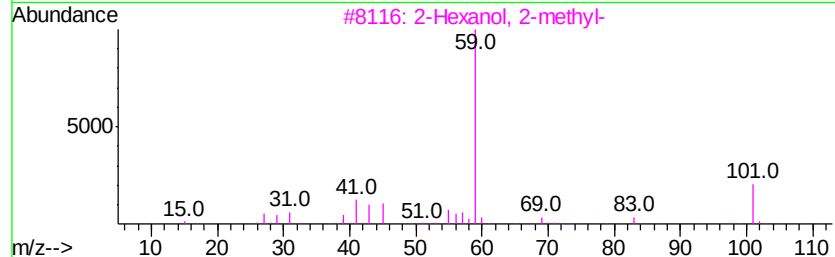
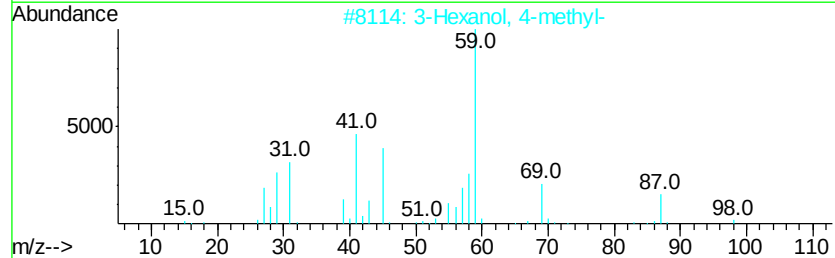
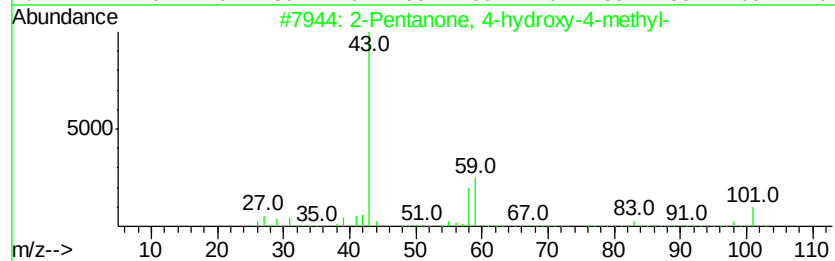
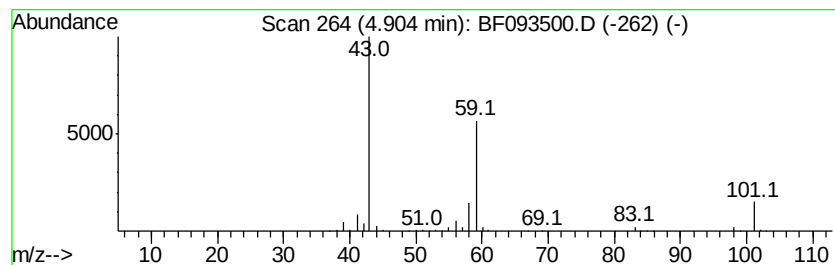
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 4.90 | 19.50 ng | 1135090 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 59   |
| 2    |    | 3-Hexanol, 4-methyl-                 | 116 | C7H16O   | 000615-29-2 | 33   |
| 3    |    | 2-Hexanol, 2-methyl-                 | 116 | C7H16O   | 000625-23-0 | 28   |
| 4    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 5    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

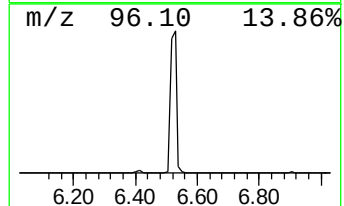
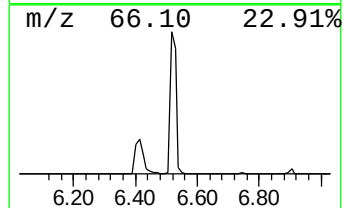
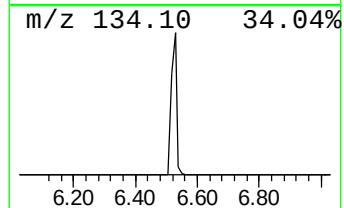
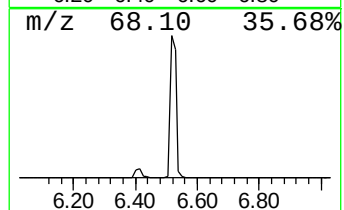
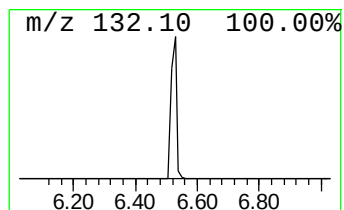
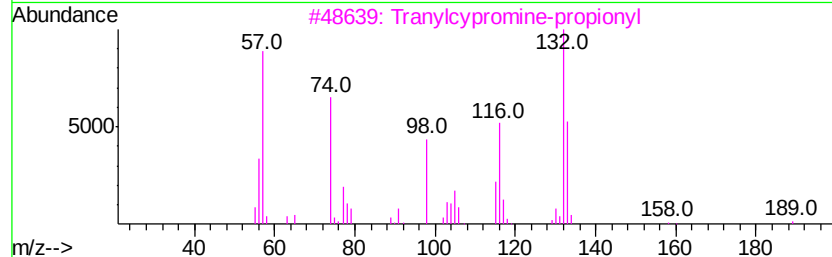
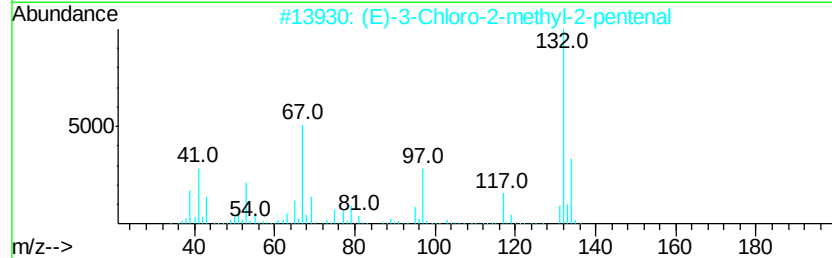
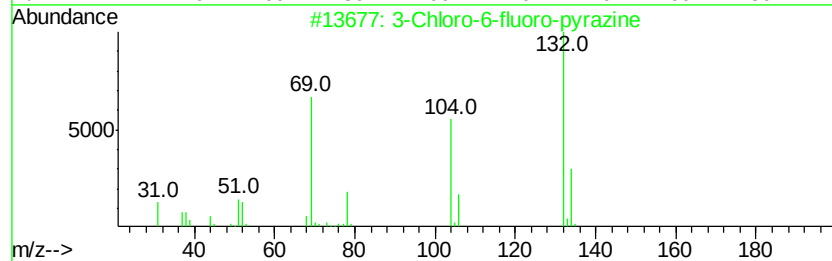
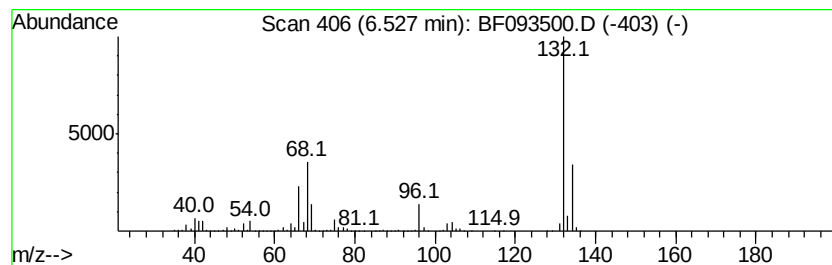
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.53 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.53 | 81.90 ng | 4768360 | 1,4-Dichlorobenzene-d4 | 6.74 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 38   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | Tranvlcypropine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 16   |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

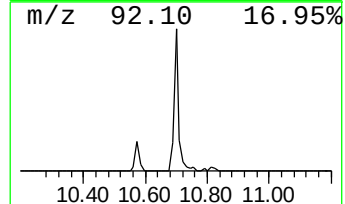
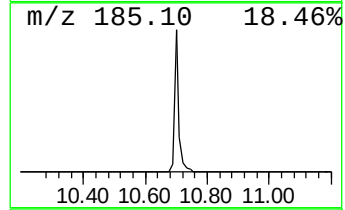
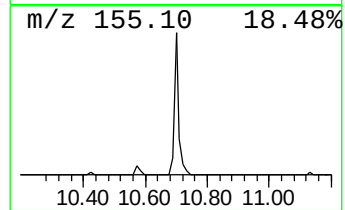
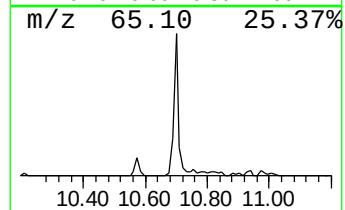
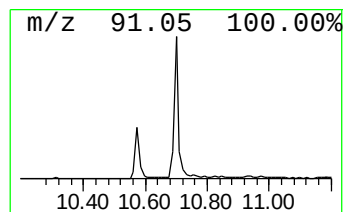
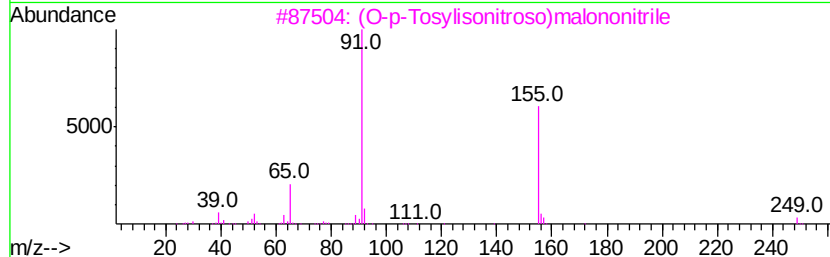
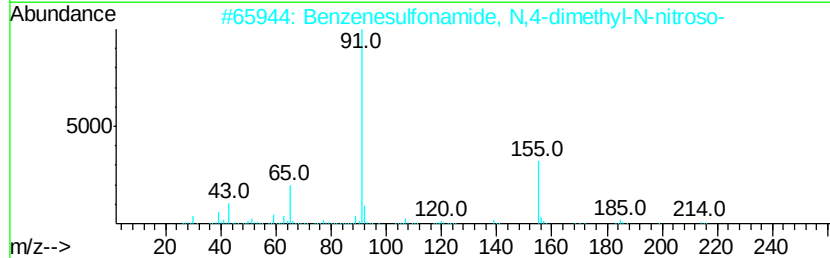
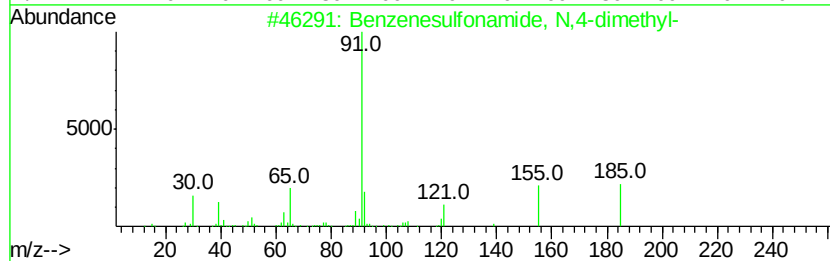
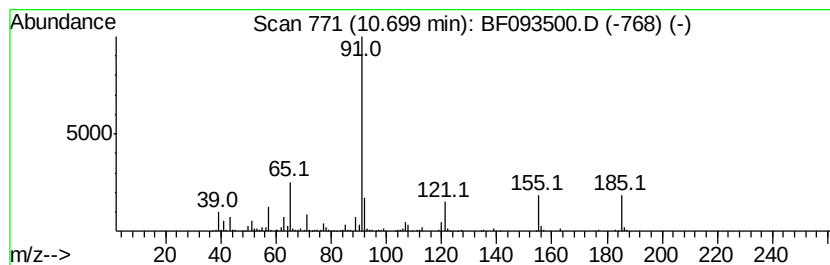
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Benzenesulfonamide, N,4-dim... Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 10.70 | 6.46 ng | 488343 | Phenanthrene-d10 | 11.27 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm      | CAS#        | Qual |
|---------|---|-------------------------------------|-----|--------------|-------------|------|
| 1       |   | Benzenesulfonamide, N,4-dimethyl-   | 185 | C8H11NO2S    | 000640-61-9 | 92   |
| 2       |   | Benzenesulfonamide, N,4-dimethyl... | 214 | C8H10N2O3S   | 000080-11-5 | 53   |
| 3       |   | (O-p-Tosylisonitroso)malononitrile  | 249 | C10H7N3O3S   | 020893-01-0 | 47   |
| 4       |   | N-Tosyloxy-2-methyl-3,3-bis(trif... | 363 | C12H11F6N03S | 055734-42-4 | 47   |
| 5       |   | 4-Toluenesulfonylmethylisocyanide   | 195 | C9H9NO2S     | 036635-61-7 | 47   |



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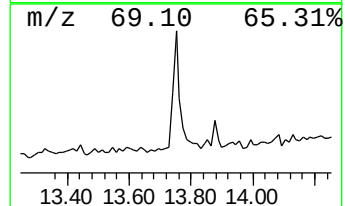
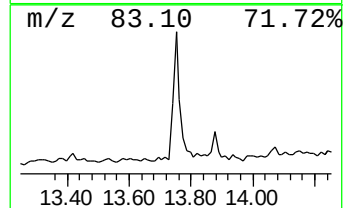
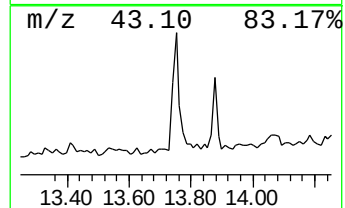
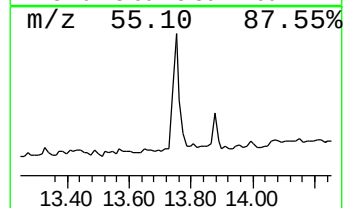
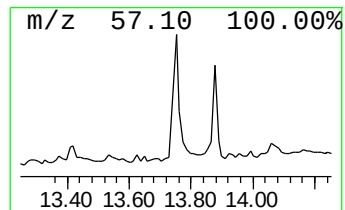
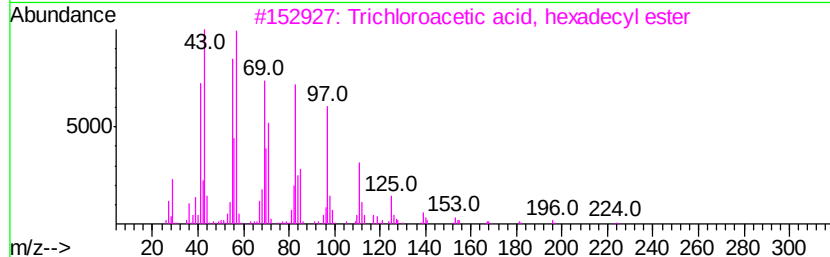
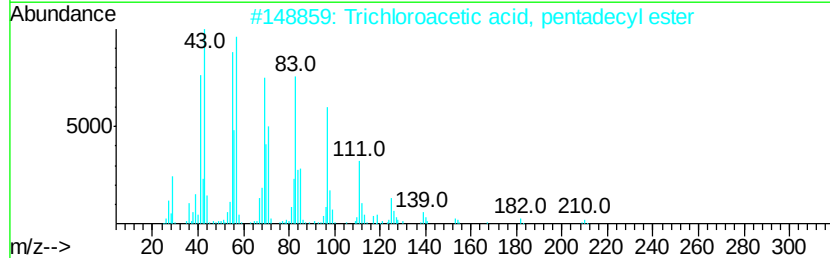
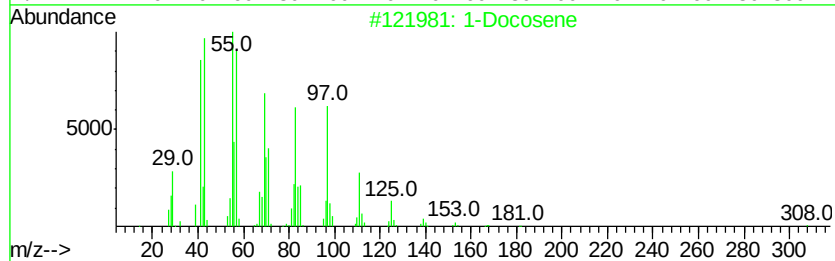
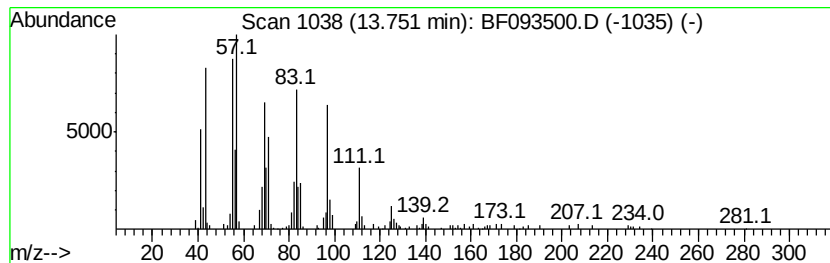
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 1-Docosene Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.75 | 5.60 ng | 283164 | Chrysene-d12     | 13.91 |

| Hit# of | 5                                   | Tentative ID | MW  | MolForm     | CAS#        | Qual |
|---------|-------------------------------------|--------------|-----|-------------|-------------|------|
| 1       | 1-Docosene                          |              | 308 | C22H44      | 001599-67-3 | 94   |
| 2       | Trichloroacetic acid, pentadecyl... |              | 372 | C17H31Cl3O2 | 074339-53-0 | 94   |
| 3       | Trichloroacetic acid, hexadecyl ... |              | 386 | C18H33Cl3O2 | 074339-54-1 | 91   |
| 4       | 3-Eicosene, (E)-                    |              | 280 | C20H40      | 074685-33-9 | 90   |
| 5       | Trichloroacetic acid, tetradecyl... |              | 358 | C16H29Cl3O2 | 074339-52-9 | 90   |



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ALS Vial : 20 Sample Multiplier: 1

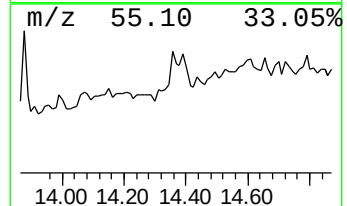
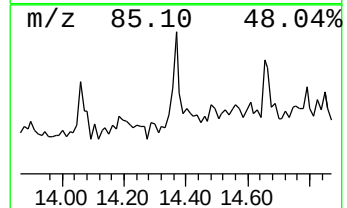
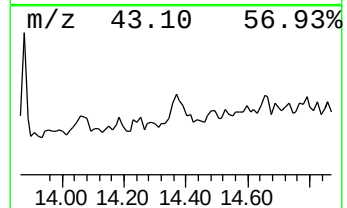
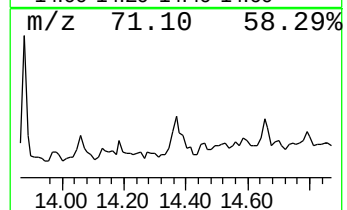
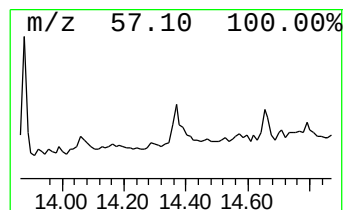
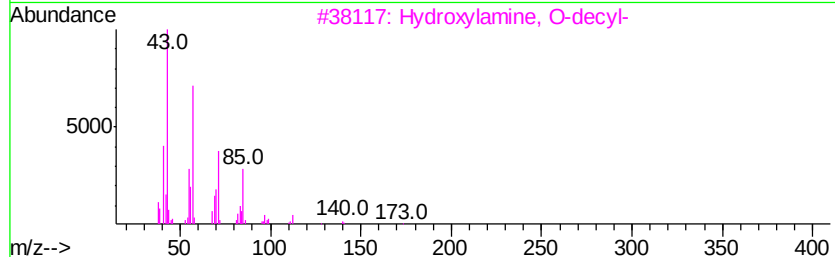
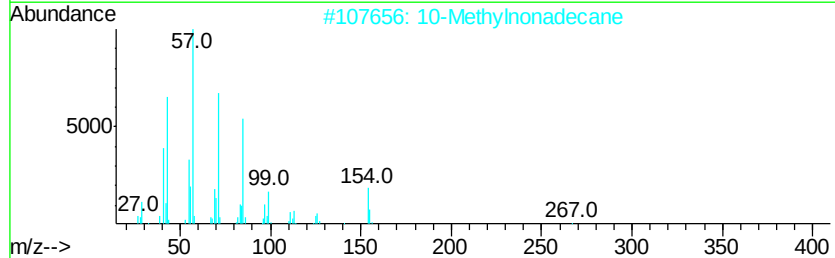
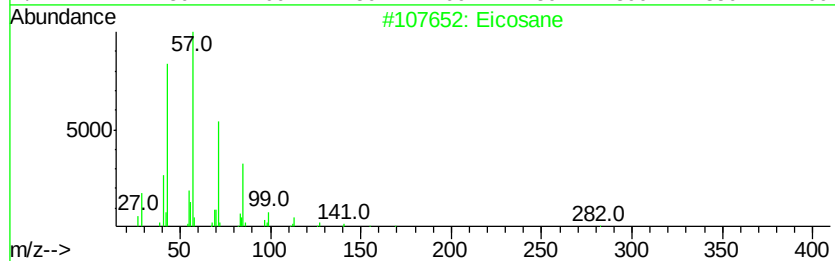
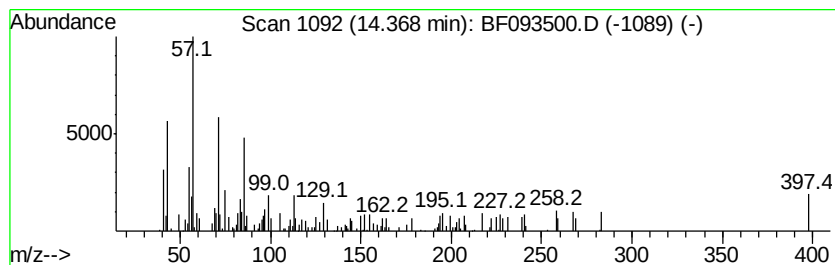
Instrument :  
BNA\_F  
ClientSampleId :  
RU-BUBBLE-01

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Eicosane Concentration Rank 7

| R.T.    | EstConc                       | Area         | Relative to ISTD | R.T.      |
|---------|-------------------------------|--------------|------------------|-----------|
| 14.37   | 2.69 ng                       | 135835       | Chrysene-d12     | 13.91     |
| Hit# of | 5                             | Tentative ID | MW MolForm       | CAS# Qual |
| 1       | Eicosane                      | 282 C20H42   | 000112-95-8      | 55        |
| 2       | 10-Methylnonadecane           | 282 C20H42   | 056862-62-5      | 46        |
| 3       | Hydroxylamine, O-decyl-       | 173 C10H23NO | 029812-79-1      | 46        |
| 4       | Heptadecane                   | 240 C17H36   | 000629-78-7      | 43        |
| 5       | Octane, 3-ethyl-2,7-dimethyl- | 170 C12H26   | 062183-55-5      | 43        |





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030917\  
Data File : BF093500.D  
Acq On : 10 Mar 2017 2:42  
Operator : SJ/MA  
Sample : I2188-02  
Misc :  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RU-BUBBLE-01

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

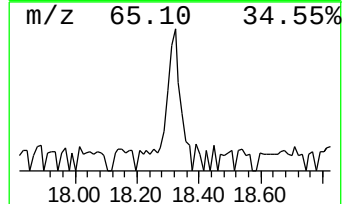
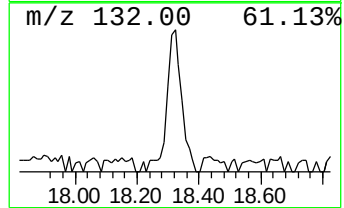
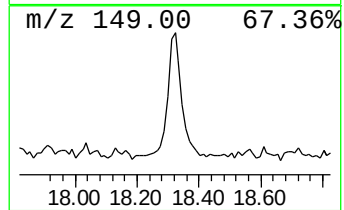
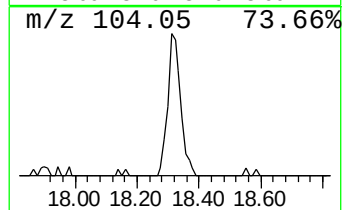
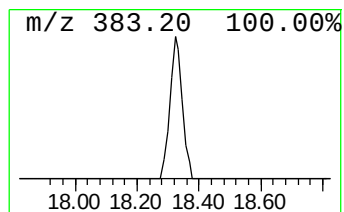
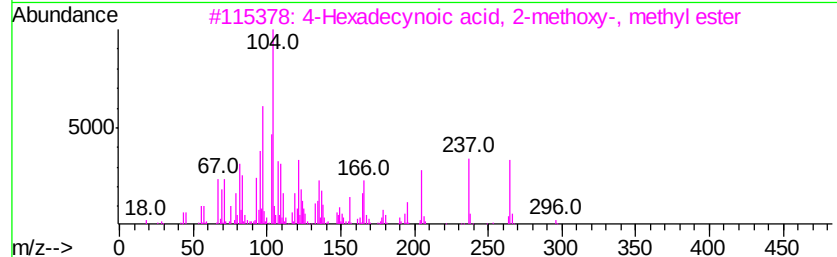
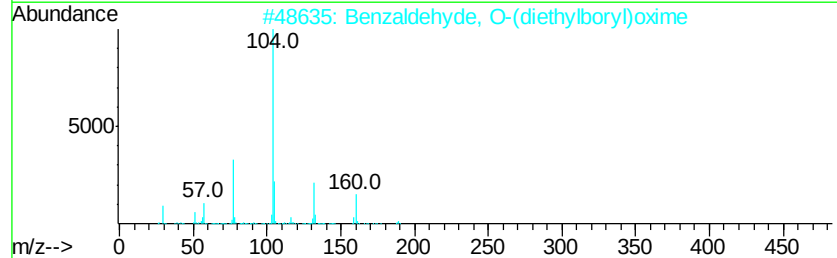
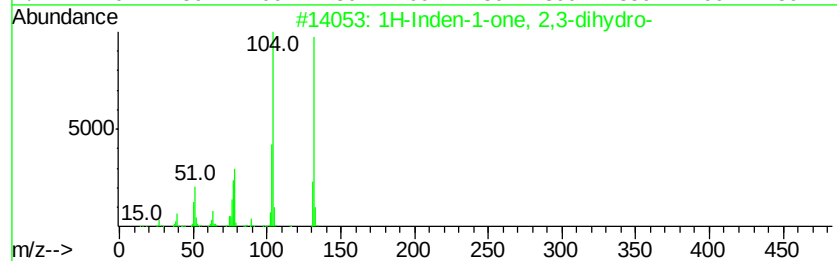
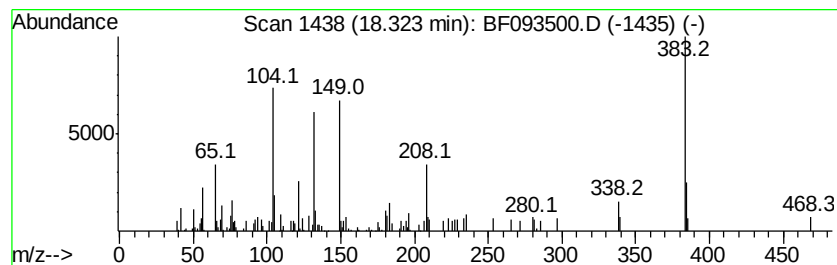
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 unknown18.32 Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.32 | 3.49 ng | 179868 | Perylene-d12     | 15.32 |

| Hit# | of | Tentative ID                         | MW  | MolForm   | CAS#        | Qual |
|------|----|--------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 1H-Inden-1-one, 2,3-dihydro-         | 132 | C9H8O     | 000083-33-0 | 22   |
| 2    |    | Benzaldehyde, O-(diethylboryl)oxime  | 189 | C11H16BN0 | 074421-33-3 | 14   |
| 3    |    | 4-Hexadecyanoic acid, 2-methoxy-,... | 296 | C18H32O3  | 040924-17-2 | 11   |
| 4    |    | 4-Pyridinecarbonitrile               | 104 | C6H4N2    | 000100-48-1 | 10   |
| 5    |    | 3-Methyl-2,6-diphenylpiperidin-4...  | 265 | C18H19N0  | 005554-57-4 | 10   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030917\  
Data File : BF093500.D  
Acq On : 10 Mar 2017 2:42  
Operator : SJ/MA  
Sample : I2188-02  
Misc :  
ALS Vial : 20 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RU-BUBBLE-01

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.90  | 19.5    | ng    | 1135090  | 1                     | 6.74  | 1164480 | 20.0 |
| unknown6.53          | 6.53  | 81.9    | ng    | 4768360  | 1                     | 6.74  | 1164480 | 20.0 |
| Benzenesulfonamid... | 10.70 | 6.5     | ng    | 488343   | 4                     | 11.27 | 1512530 | 20.0 |
| 1-Docosene           | 13.75 | 5.6     | ng    | 283164   | 5                     | 13.91 | 1011210 | 20.0 |
| Eicosane             | 14.37 | 2.7     | ng    | 135835   | 5                     | 13.91 | 1011210 | 20.0 |
| unknown18.32         | 18.32 | 3.5     | ng    | 179868   | 6                     | 15.32 | 1032230 | 20.0 |