

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\  
 Data File : BF095858.D  
 Acq On : 10 Jun 2017 20:44  
 Operator : SJ/MA  
 Sample : I3566-12  
 Misc :  
 ALS Vial : 13 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-07-COMP(0-4.0)

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-BF060517.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         | 2.387       | 132           | 136         | 146          | rBV      | 21762          | 51077         | 1.44%           | 0.263%        |
| 2         | 3.534       | 318           | 331         | 356          | rBV      | 1232224        | 3551764       | 100.00%         | 18.299%       |
| 3         | 4.604       | 497           | 513         | 516          | rBV      | 994517         | 3134523       | 88.25%          | 16.149%       |
| 4         | 5.269       | 623           | 626         | 655          | rBV      | 233345         | 628842        | 17.71%          | 3.240%        |
| 5         | 6.922       | 904           | 907         | 921          | rBV      | 670642         | 1157493       | 32.59%          | 5.963%        |
| 6         | 7.022       | 921           | 924         | 939          | rVB      | 580831         | 976290        | 27.49%          | 5.030%        |
| 7         | 7.369       | 979           | 983         | 998          | rVB      | 295780         | 403315        | 11.36%          | 2.078%        |
| 8         | 7.604       | 1018          | 1023        | 1038         | rBV      | 937661         | 1206835       | 33.98%          | 6.218%        |
| 9         | 8.286       | 1134          | 1139        | 1162         | rBV      | 593647         | 920586        | 25.92%          | 4.743%        |
| 10        | 9.398       | 1324          | 1328        | 1345         | rBV      | 399764         | 559236        | 15.75%          | 2.881%        |
| 11        | 11.180      | 1625          | 1631        | 1651         | rBV      | 1492786        | 1892403       | 53.28%          | 9.750%        |
| 12        | 11.874      | 1745          | 1749        | 1760         | rBV      | 116848         | 168865        | 4.75%           | 0.870%        |
| 13        | 12.222      | 1803          | 1808        | 1813         | rBV2     | 470154         | 614465        | 17.30%          | 3.166%        |
| 14        | 13.074      | 1947          | 1953        | 1960         | rBV      | 27349          | 35937         | 1.01%           | 0.185%        |
| 15        | 13.521      | 2025          | 2029        | 2043         | rBV      | 157684         | 277918        | 7.82%           | 1.432%        |
| 16        | 13.845      | 2080          | 2084        | 2094         | rBV      | 30682          | 55653         | 1.57%           | 0.287%        |
| 17        | 14.615      | 2211          | 2215        | 2220         | rVV      | 443625         | 604085        | 17.01%          | 3.112%        |
| 18        | 14.663      | 2220          | 2223        | 2232         | rVB2     | 57956          | 82892         | 2.33%           | 0.427%        |
| 19        | 15.257      | 2319          | 2324        | 2329         | rBV      | 84951          | 104041        | 2.93%           | 0.536%        |
| 20        | 16.439      | 2523          | 2525        | 2532         | rVB      | 34947          | 40636         | 1.14%           | 0.209%        |
| 21        | 16.745      | 2573          | 2577        | 2582         | rBV      | 45554          | 59433         | 1.67%           | 0.306%        |
| 22        | 16.992      | 2613          | 2619        | 2625         | rBV      | 1259155        | 1564402       | 44.05%          | 8.060%        |
| 23        | 17.656      | 2728          | 2732        | 2735         | rBV      | 39353          | 45304         | 1.28%           | 0.233%        |
| 24        | 18.245      | 2828          | 2832        | 2840         | rBV3     | 73718          | 121328        | 3.42%           | 0.625%        |
| 25        | 18.333      | 2842          | 2847        | 2856         | rVV      | 407039         | 521316        | 14.68%          | 2.686%        |
| 26        | 18.403      | 2856          | 2859        | 2864         | rVB      | 61335          | 70236         | 1.98%           | 0.362%        |
| 27        | 19.368      | 3019          | 3023        | 3028         | rBV      | 55400          | 63236         | 1.78%           | 0.326%        |
| 28        | 19.609      | 3061          | 3064        | 3069         | rBV2     | 24469          | 37031         | 1.04%           | 0.191%        |
| 29        | 19.997      | 3126          | 3130        | 3141         | rBV      | 316544         | 460565        | 12.97%          | 2.373%        |

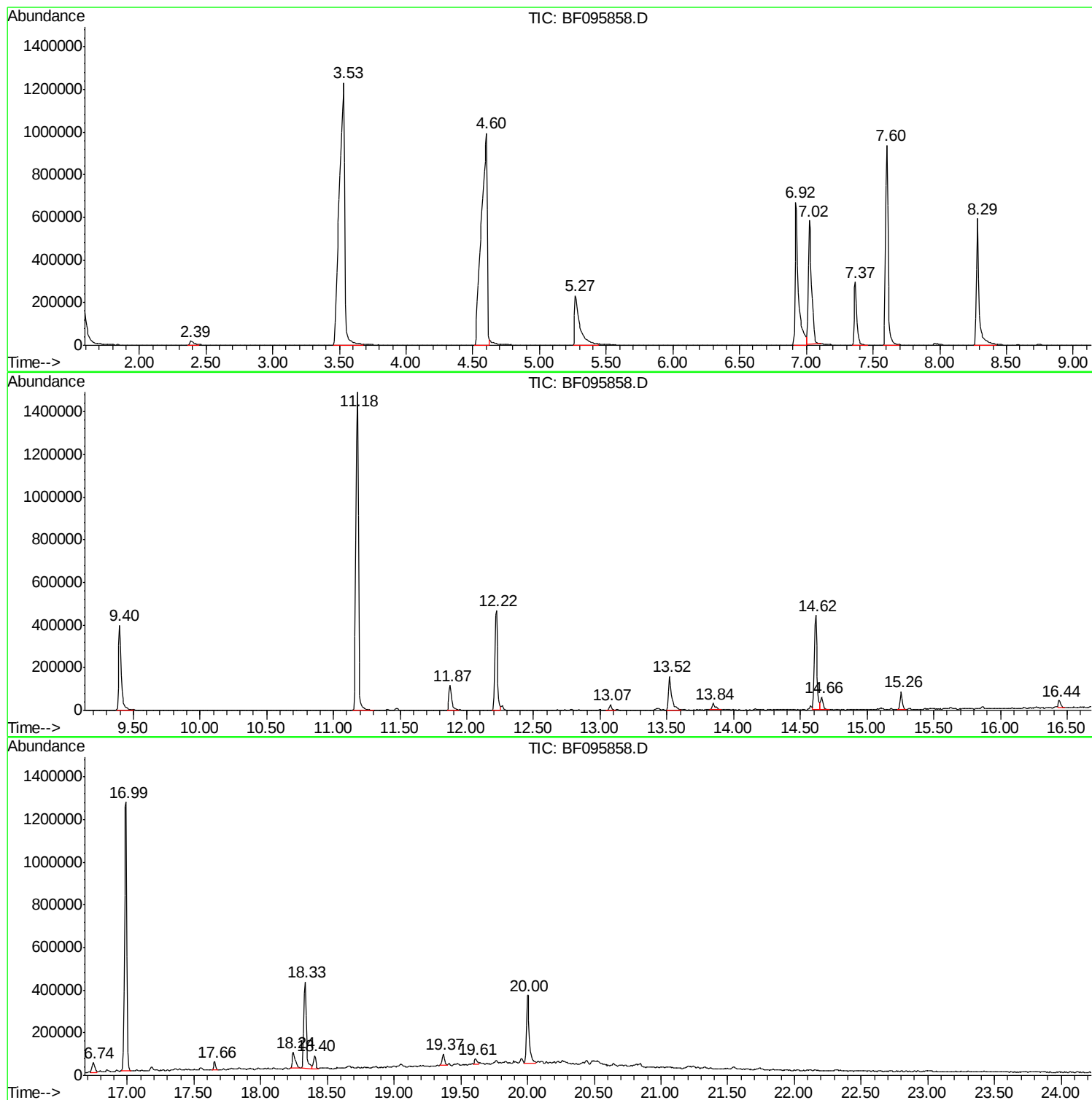
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SB-07-COMP(0-4.0)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.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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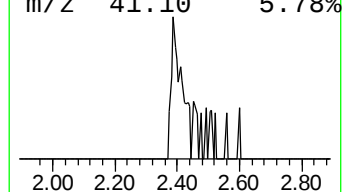
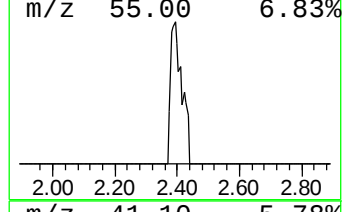
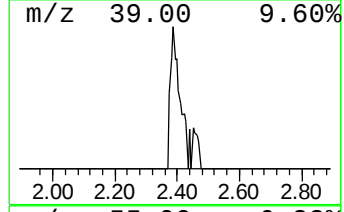
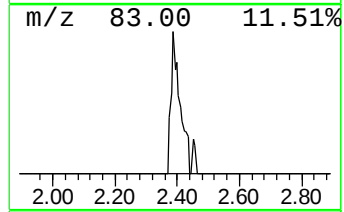
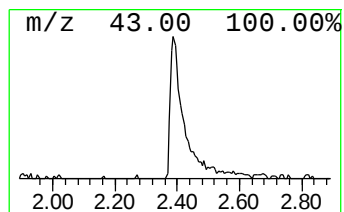
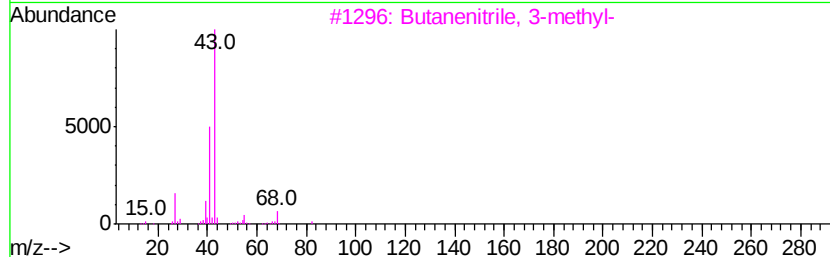
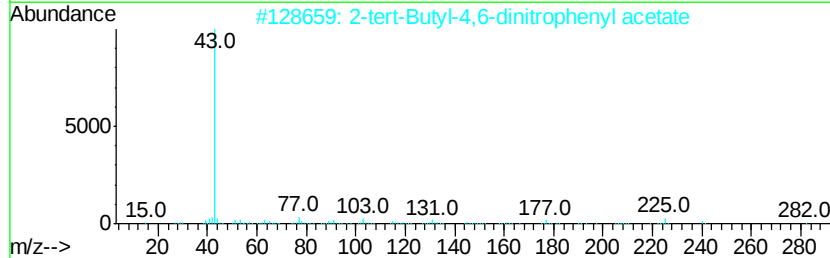
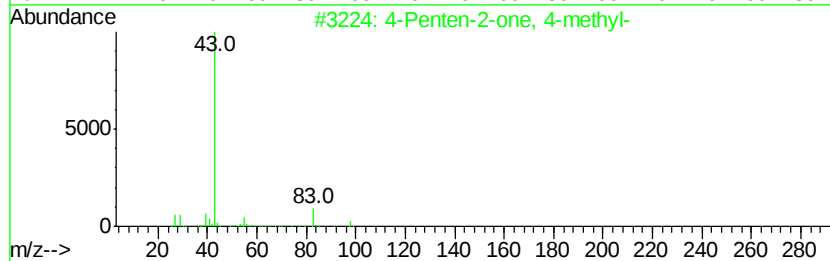
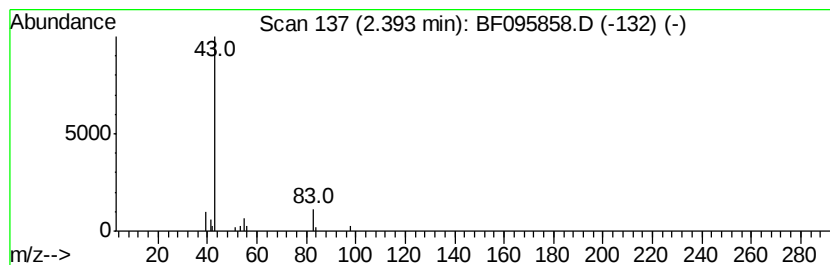
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown2.39 Concentration Rank 8

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 2.39 | 2.53 ng | 51077 | 1,4-Dichlorobenzene-d4 | 7.37 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 4-Penten-2-one, 4-methyl-           | 98  | C6H10O     | 003744-02-3  | 9    |
| 2    |    |   | 2-tert-Butyl-4,6-dinitrophenyl a... | 282 | C12H14N2O6 | 1000373-33-1 | 2    |
| 3    |    |   | Butanenitrile, 3-methyl-            | 83  | C5H9N      | 000625-28-5  | 2    |
| 4    |    |   | Hydrogen azide                      | 43  | HN3        | 007782-79-8  | 2    |
| 5    |    |   | Pent-3-enylamine                    | 85  | C5H11N     | 087156-70-5  | 2    |



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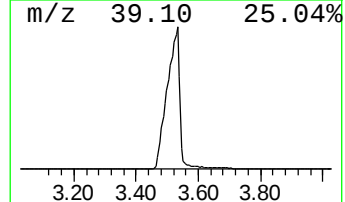
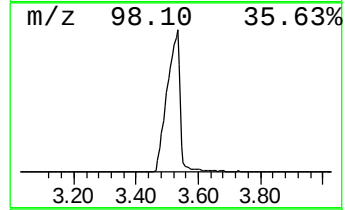
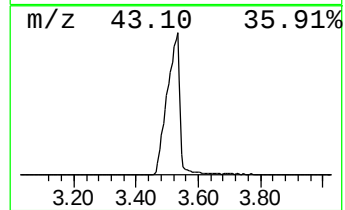
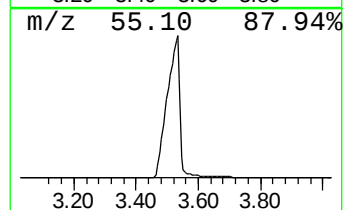
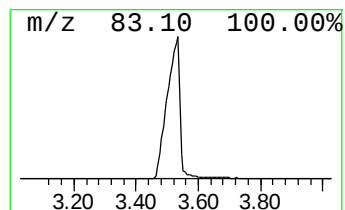
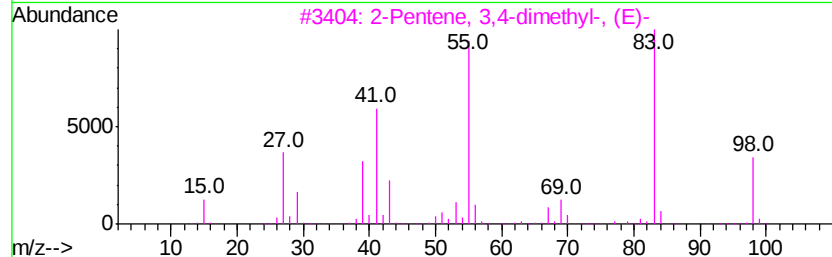
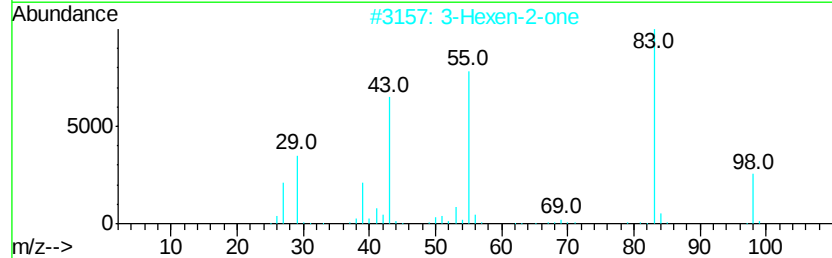
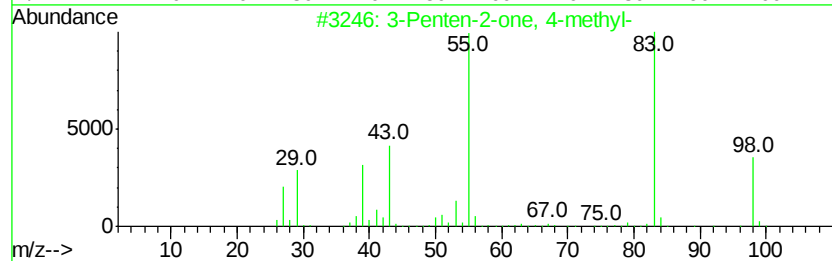
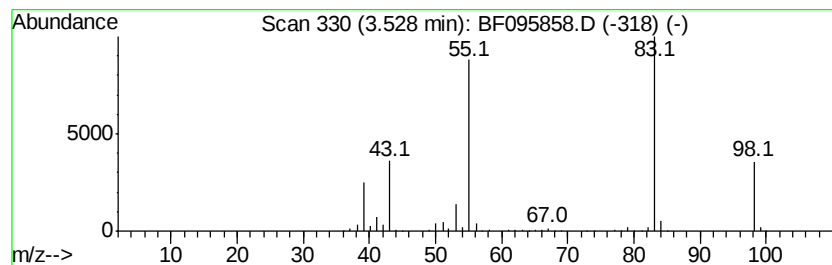
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 3.53 | 176.13 ng | 3551760 | 1,4-Dichlorobenzene-d4 | 7.37 |

| Hit# | of | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|--------------------------------|----|---------|-------------|------|
| 1    | 5  | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 95   |
| 2    |    | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 91   |
| 3    |    | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 90   |
| 4    |    | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 5    |    | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 80   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

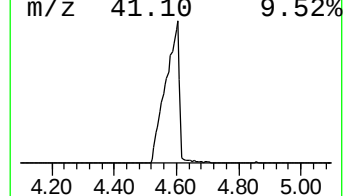
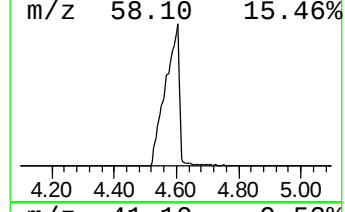
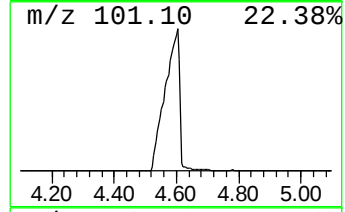
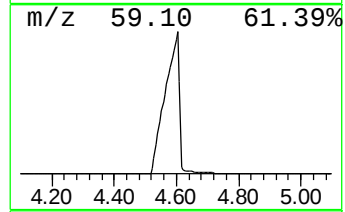
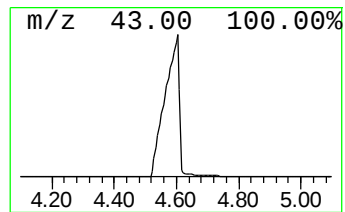
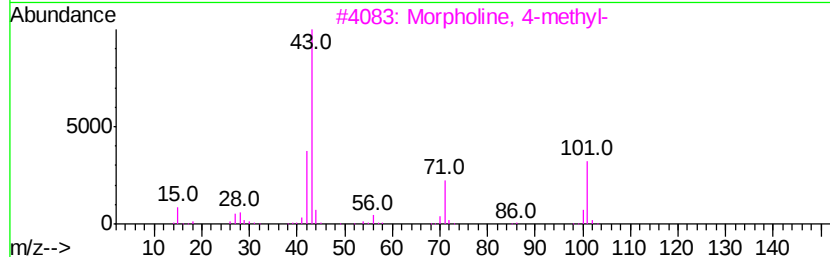
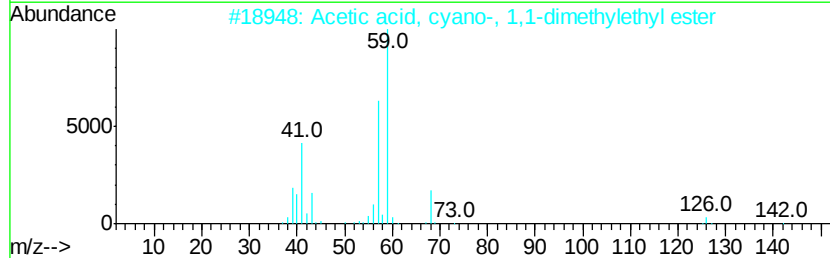
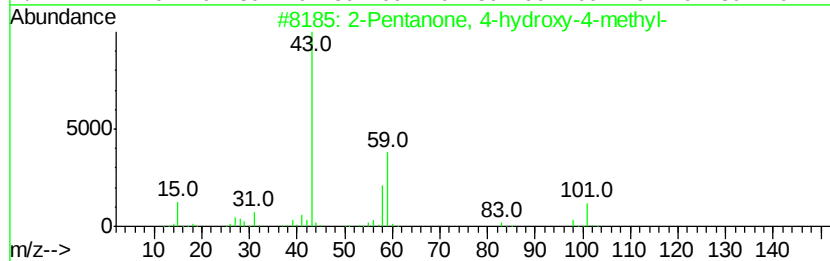
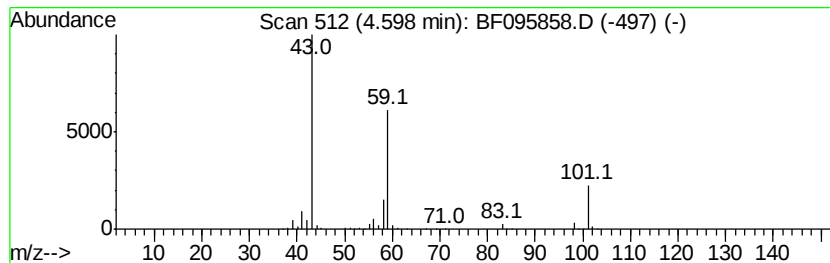
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 4.60 | 155.44 ng | 3134520 | 1,4-Dichlorobenzene-d4 | 7.37 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 25   |
| 3    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |
| 4    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | 5-Hexen-2-one                        | 98  | C6H10O   | 000109-49-9 | 9    |



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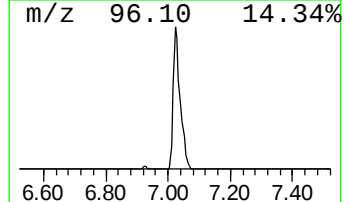
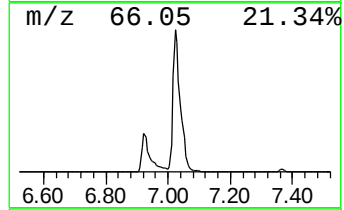
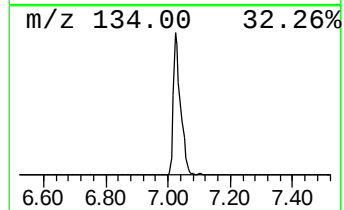
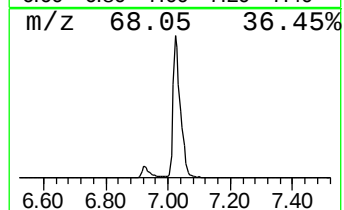
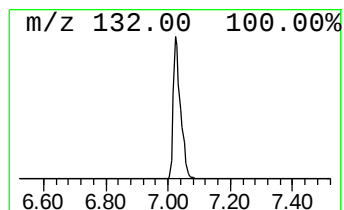
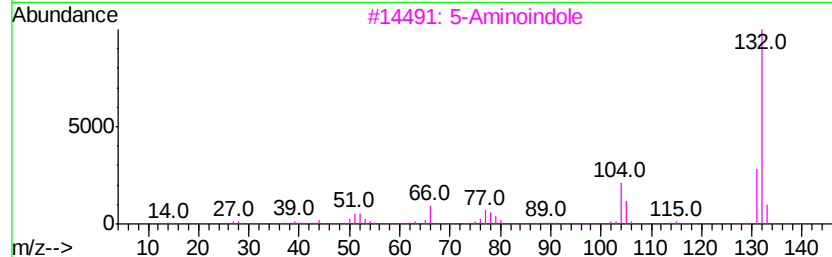
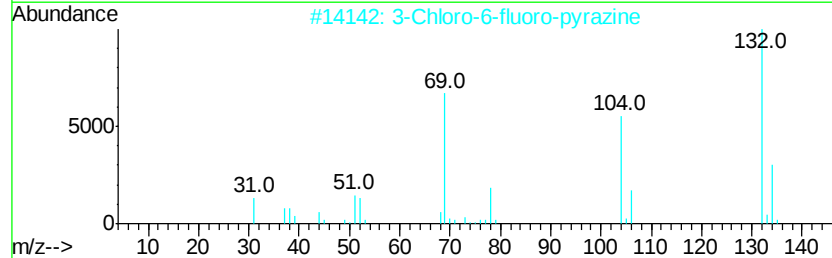
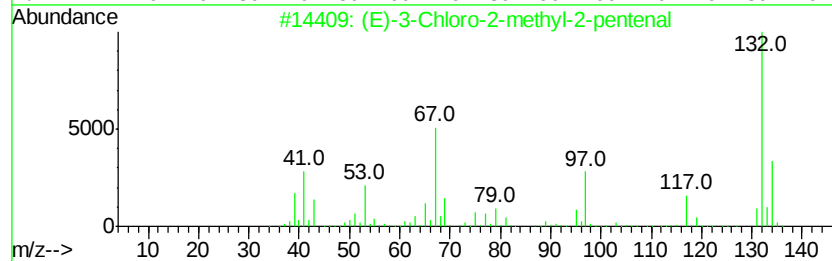
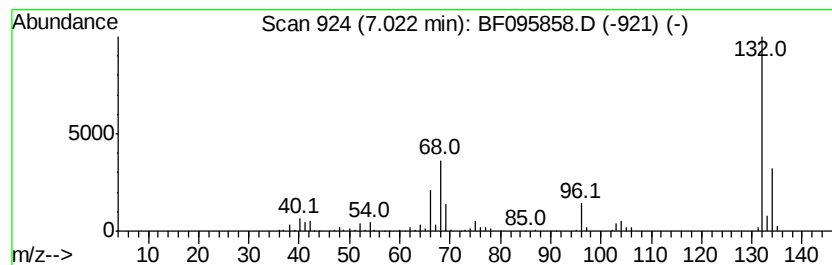
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
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\*\*\*\*\*  
Peak Number 4 unknown7.02 Concentration Rank 4

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 7.02 | 48.41 ng | 976290 | 1,4-Dichlorobenzene-d4 | 7.37 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 35   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 10   |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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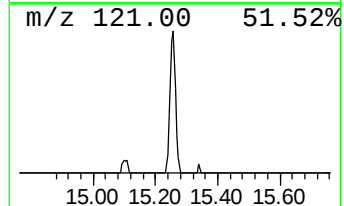
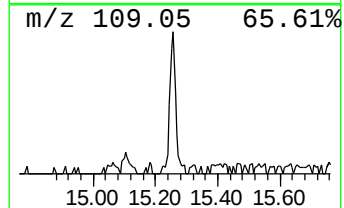
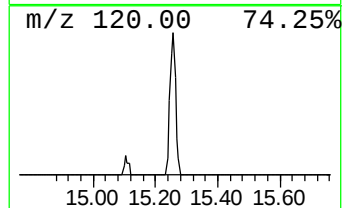
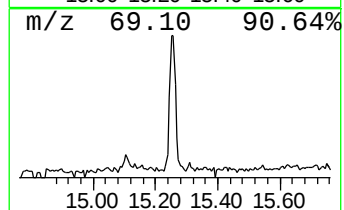
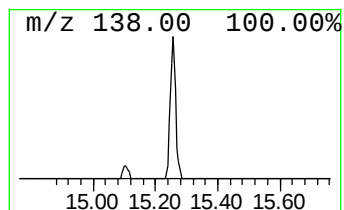
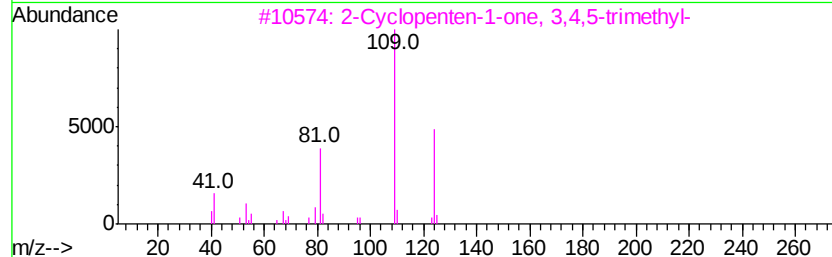
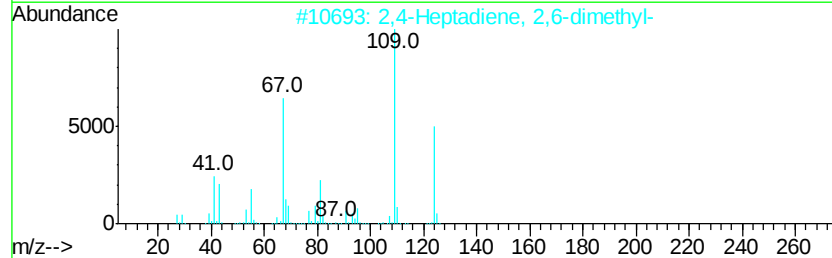
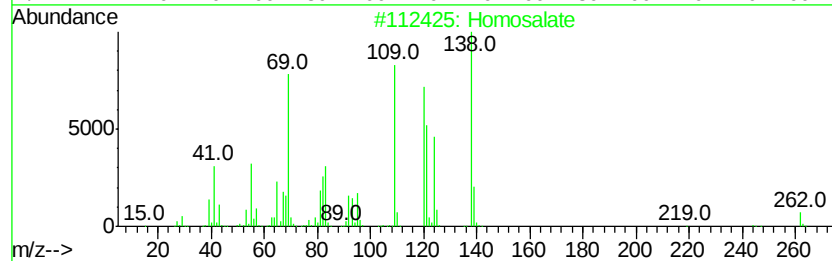
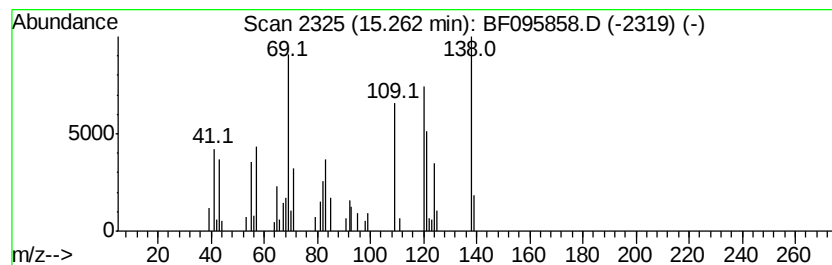
Instrument :  
BNA\_F  
ClientSampleId :  
SB-07-COMP(0-4.0)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 Homosalate Concentration Rank 6

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 15.26     | 3.44 ng                             | 104041 | Phenanthrene-d10 | 14.62       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | Homosalate                          | 262    | C16H22O3         | 000118-56-9 | 50   |
| 2         | 2,4-Heptadiene, 2,6-dimethyl-       | 124    | C9H16            | 004634-87-1 | 14   |
| 3         | 2-Cyclopenten-1-one, 3,4,5-trime... | 124    | C8H12O           | 055683-21-1 | 14   |
| 4         | n-Hexyl-4-hydroxybenzoate           | 222    | C13H18O3         | 001083-27-8 | 14   |
| 5         | 2,6-Pyridinediamine                 | 109    | C5H7N3           | 000141-86-6 | 11   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061017\  
Data File : BF095858.D  
Acq On : 10 Jun 2017 20:44  
Operator : SJ/MA  
Sample : I3566-12  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-07-COMP(0-4.0)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

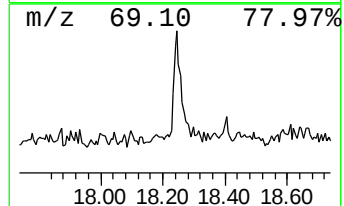
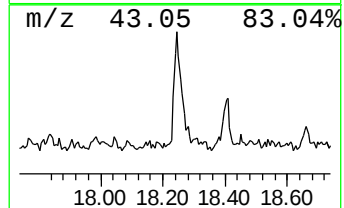
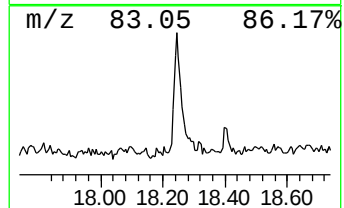
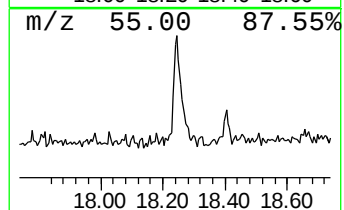
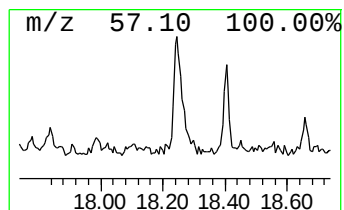
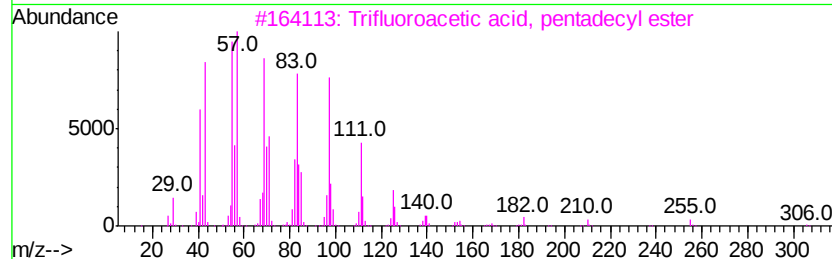
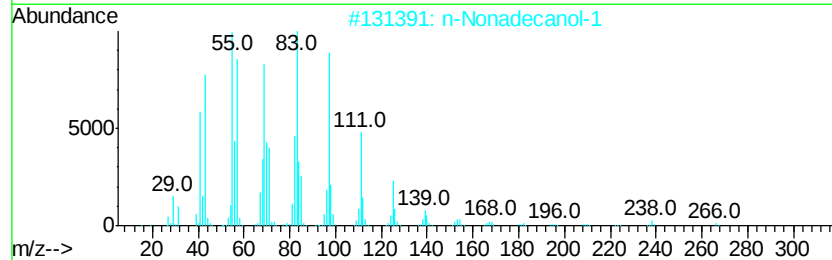
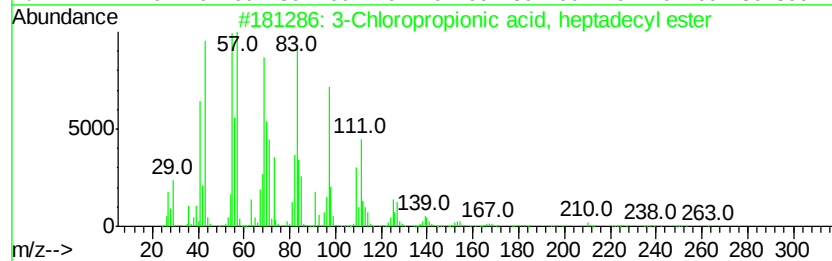
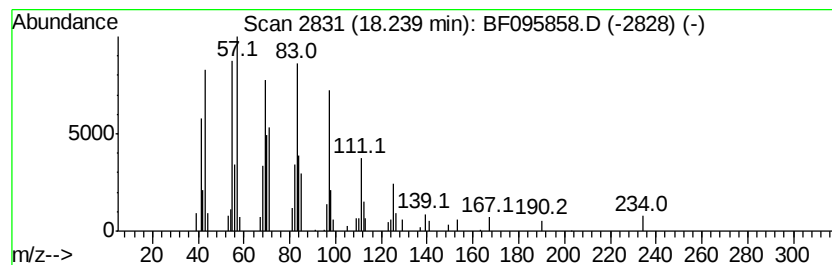
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 3-Chloropropionic acid, hep... Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.24 | 4.65 ng | 121328 | Chrysene-d12     | 18.33 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2  | 1000283-05-1 | 91   |
| 2    |    | n-Nonadecanol-1                     | 284 | C19H40O     | 001454-84-8  | 91   |
| 3    |    | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2  | 959010-23-2  | 90   |
| 4    |    | 1-Heneicosanol                      | 312 | C21H44O     | 015594-90-8  | 87   |
| 5    |    | Trichloroacetic acid, pentadecyl... | 372 | C17H31Cl3O2 | 074339-53-0  | 87   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061017\  
Data File : BF095858.D  
Acq On : 10 Jun 2017 20:44  
Operator : SJ/MA  
Sample : I3566-12  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-07-COMP(0-4.0)

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF060517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

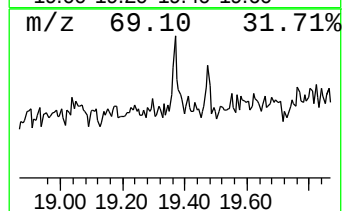
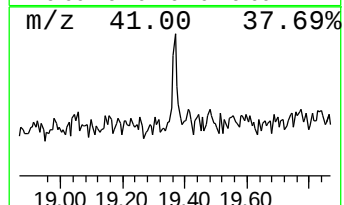
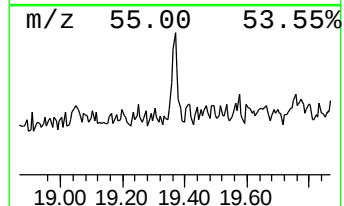
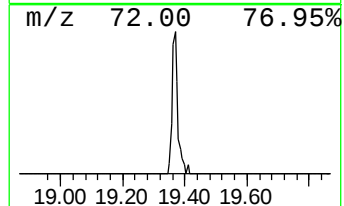
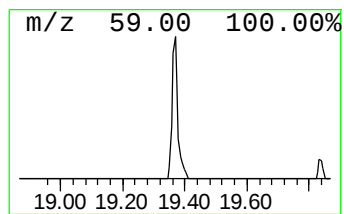
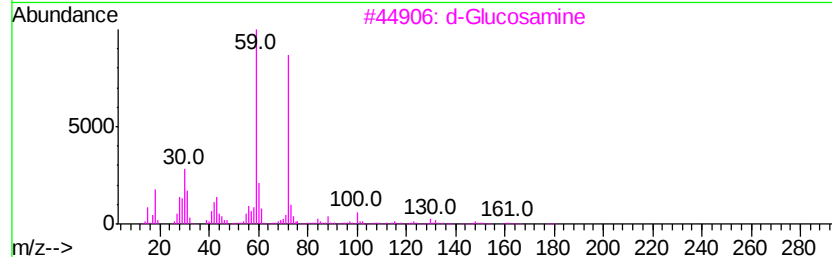
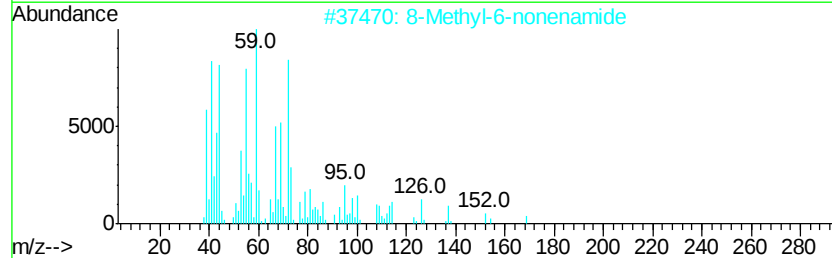
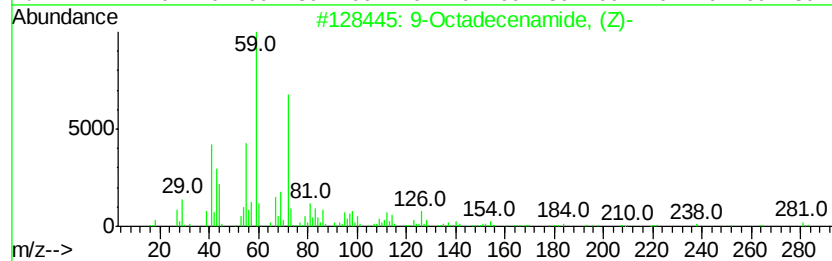
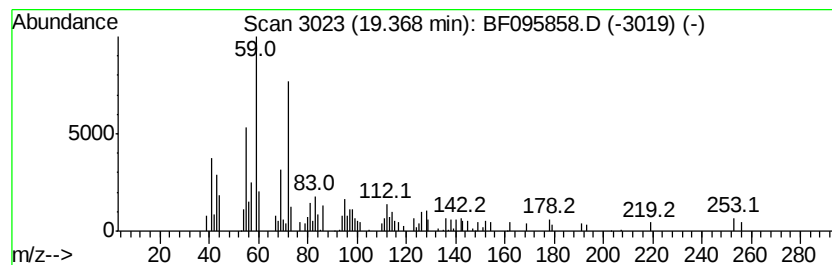
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 9-Octadecenamide, (Z)- Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 19.37 | 2.75 ng | 63236 | Perylene-d12     | 20.00 |

| Hit# | of | Tentative ID               | MW  | MolForm    | CAS#         | Qual |
|------|----|----------------------------|-----|------------|--------------|------|
| 1    | 5  | 9-Octadecenamide, (Z)-     | 281 | C18H35NO   | 000301-02-0  | 80   |
| 2    |    | 8-Methyl-6-nonenamide      | 169 | C10H19NO   | 1000293-20-9 | 72   |
| 3    |    | d-Glucosamine              | 179 | C6H13NO5   | 000090-77-7  | 53   |
| 4    |    | Pentadecanamide, 15-bromo- | 319 | C15H30BrNO | 1000163-86-1 | 47   |
| 5    |    | Hexadecanamide             | 255 | C16H33NO   | 000629-54-9  | 47   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061017\  
Data File : BF095858.D  
Acq On : 10 Jun 2017 20:44  
Operator : SJ/MA  
Sample : I3566-12  
Misc :  
ALS Vial : 13 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-07-COMP(0-4.0)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF060517.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 |
| unknown2.39          | 2.39  | 2.5     | ng    | 51077    | 1                     | 7.37  | 403315 | 20.0 |
| 3-Penten-2-one, 4... | 3.53  | 176.1   | ng    | 3551760  | 1                     | 7.37  | 403315 | 20.0 |
| 2-Pentanone, 4-hy... | 4.60  | 155.4   | ng    | 3134520  | 1                     | 7.37  | 403315 | 20.0 |
| unknown7.02          | 7.02  | 48.4    | ng    | 976290   | 1                     | 7.37  | 403315 | 20.0 |
| Homosalate           | 15.26 | 3.4     | ng    | 104041   | 4                     | 14.62 | 604085 | 20.0 |
| 3-Chloropropionic... | 18.24 | 4.7     | ng    | 121328   | 5                     | 18.33 | 521316 | 20.0 |
| 9-Octadecenamide,... | 19.37 | 2.8     | ng    | 63236    | 6                     | 20.00 | 460565 | 20.0 |