

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
 Data File : BF101505.D  
 Acq On : 19 Dec 2017 3:50  
 Operator : SJ/JU  
 Sample : I6909-07  
 Misc :  
 ALS Vial : 32 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 121217-TIDO-E-U-B

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-BF121417.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         | 5.022       | 496           | 499         | 512          | rBV      | 87075          | 117505        | 3.94%           | 0.585%        |
| 2         | 5.434       | 566           | 569         | 589          | rBV      | 823910         | 1125422       | 37.77%          | 5.606%        |
| 3         | 6.457       | 740           | 743         | 761          | rBV2     | 531167         | 758761        | 25.46%          | 3.780%        |
| 4         | 6.581       | 761           | 764         | 777          | rVV      | 1736784        | 1843531       | 61.87%          | 9.184%        |
| 5         | 6.810       | 799           | 803         | 811          | rBV      | 830871         | 728974        | 24.46%          | 3.631%        |
| 6         | 6.963       | 825           | 829         | 847          | rBV      | 2544096        | 2495171       | 83.74%          | 12.430%       |
| 7         | 7.381       | 895           | 900         | 910          | rBV      | 1862769        | 1915514       | 64.28%          | 9.542%        |
| 8         | 8.092       | 1017          | 1021        | 1038         | rVB      | 906960         | 857553        | 28.78%          | 4.272%        |
| 9         | 9.169       | 1199          | 1204        | 1207         | rBV      | 3009173        | 2979816       | 100.00%         | 14.844%       |
| 10        | 9.563       | 1264          | 1271        | 1280         | rBV      | 74357          | 74385         | 2.50%           | 0.371%        |
| 11        | 9.851       | 1316          | 1320        | 1329         | rVB      | 744649         | 748976        | 25.13%          | 3.731%        |
| 12        | 10.563      | 1438          | 1441        | 1447         | rBV      | 35273          | 34756         | 1.17%           | 0.173%        |
| 13        | 10.645      | 1451          | 1455        | 1464         | rBV      | 993745         | 997909        | 33.49%          | 4.971%        |
| 14        | 11.339      | 1569          | 1573        | 1581         | rBV      | 729626         | 682959        | 22.92%          | 3.402%        |
| 15        | 11.810      | 1648          | 1653        | 1657         | rBV5     | 26777          | 51425         | 1.73%           | 0.256%        |
| 16        | 11.857      | 1657          | 1661        | 1671         | rVV2     | 128820         | 182625        | 6.13%           | 0.910%        |
| 17        | 12.310      | 1735          | 1738        | 1747         | rBV8     | 24861          | 46463         | 1.56%           | 0.231%        |
| 18        | 12.563      | 1777          | 1781        | 1789         | rBV4     | 66754          | 115728        | 3.88%           | 0.577%        |
| 19        | 12.639      | 1792          | 1794        | 1800         | rVB6     | 28545          | 33150         | 1.11%           | 0.165%        |
| 20        | 12.727      | 1807          | 1809        | 1817         | rVB6     | 27277          | 35431         | 1.19%           | 0.177%        |
| 21        | 12.921      | 1838          | 1842        | 1846         | rBV      | 2397836        | 2352721       | 78.96%          | 11.720%       |
| 22        | 12.969      | 1846          | 1850        | 1853         | rVB5     | 38621          | 48318         | 1.62%           | 0.241%        |
| 23        | 13.804      | 1989          | 1992        | 1996         | rVB2     | 63022          | 59711         | 2.00%           | 0.297%        |
| 24        | 13.992      | 2020          | 2024        | 2028         | rBV      | 797881         | 750482        | 25.19%          | 3.739%        |
| 25        | 15.462      | 2270          | 2274        | 2281         | rVB      | 495863         | 649616        | 21.80%          | 3.236%        |
| 26        | 15.680      | 2305          | 2311        | 2312         | rBV3     | 214274         | 386749        | 12.98%          | 1.927%        |

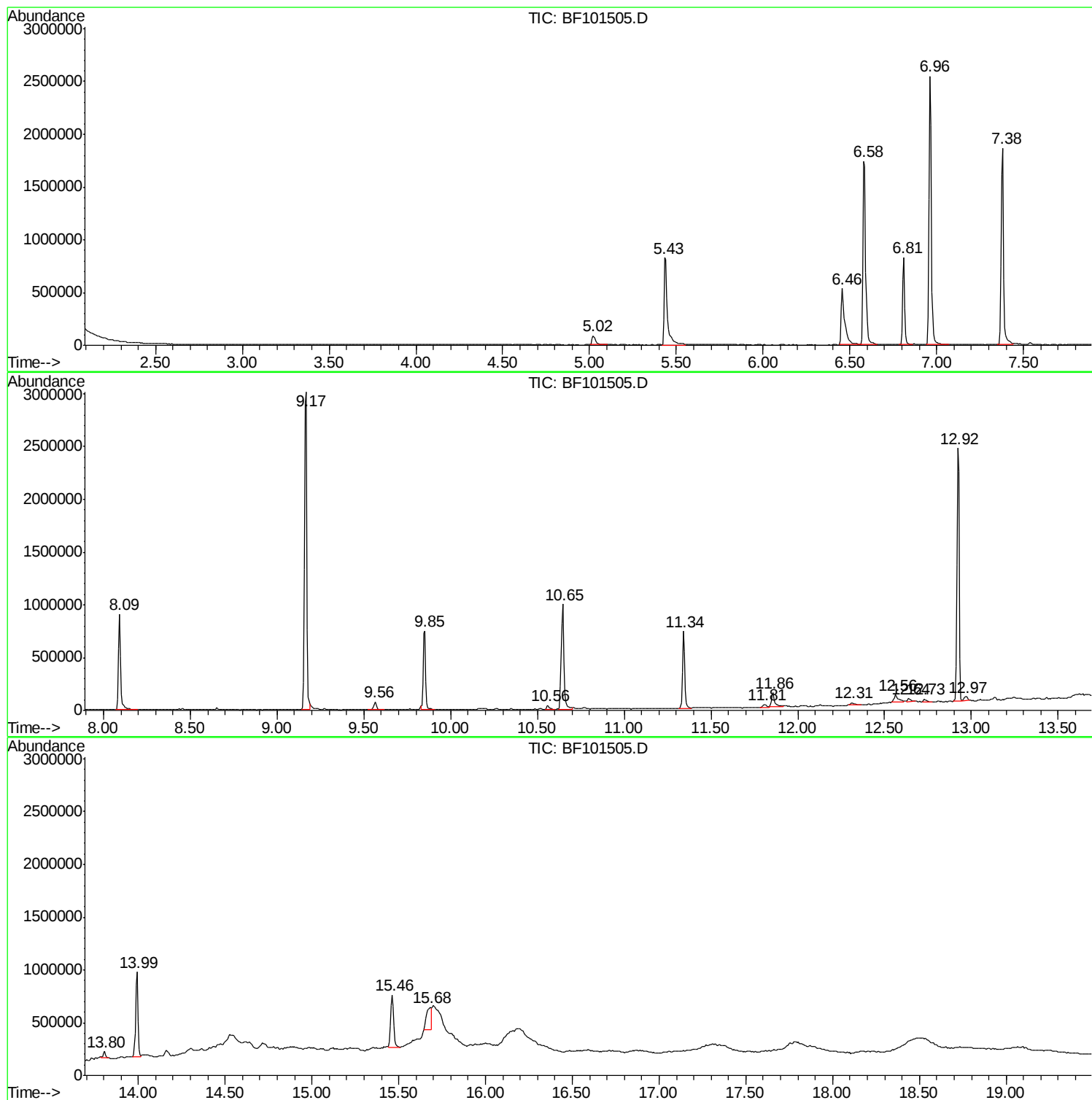
Sum of corrected areas: 20073651

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

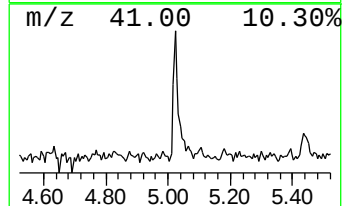
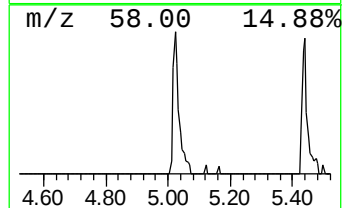
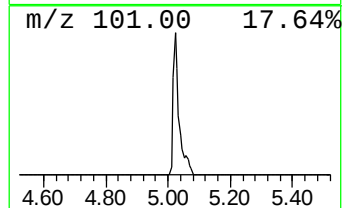
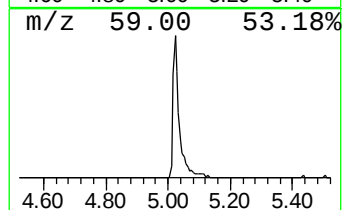
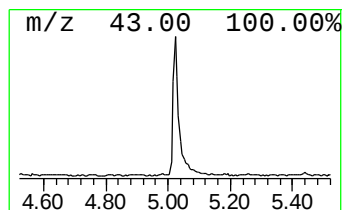
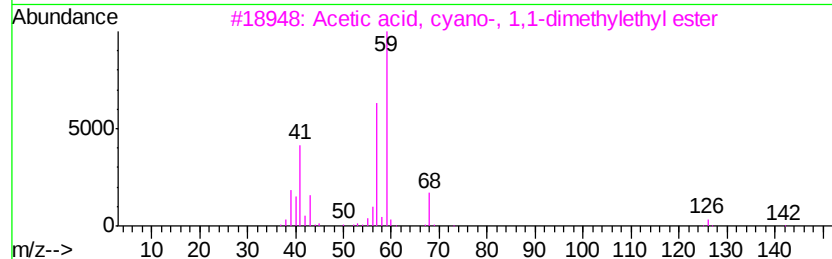
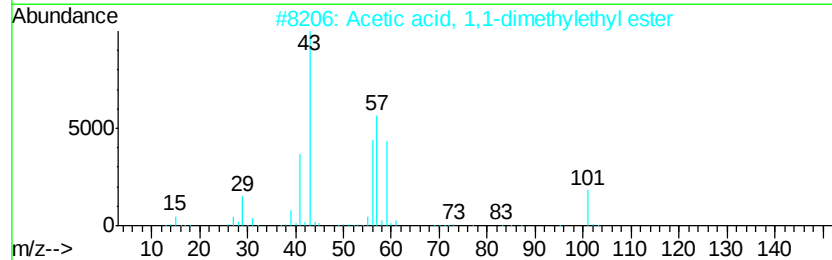
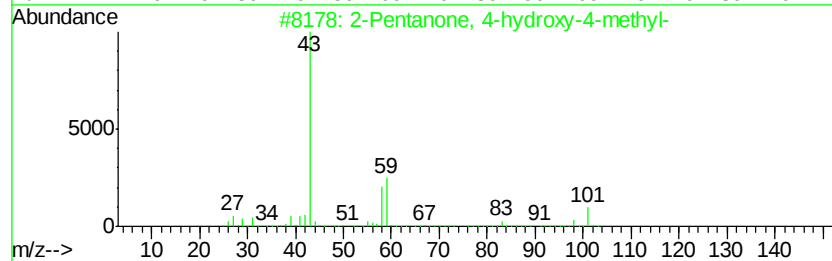
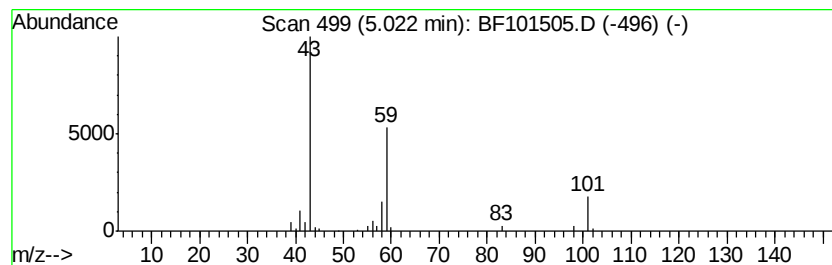
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.02 | 3.22 ng | 117505 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of | 5                                   | Tentative ID | MW       | MolForm     | CAS# | Qual |
|---------|-------------------------------------|--------------|----------|-------------|------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-    | 116          | C6H12O2  | 000123-42-2 | 45   |      |
| 2       | Acetic acid, 1,1-dimethylethyl e... | 116          | C6H12O2  | 000540-88-5 | 38   |      |
| 3       | Acetic acid, cyano-, 1,1-dimethy... | 141          | C7H11NO2 | 001116-98-9 | 25   |      |
| 4       | Morpholine, 4-methyl-               | 101          | C5H11NO  | 000109-02-4 | 9    |      |
| 5       | Acetamide, N-(aminocarbonyl)-       | 102          | C3H6N2O2 | 000591-07-1 | 9    |      |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

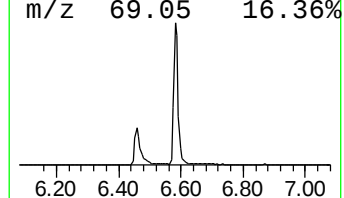
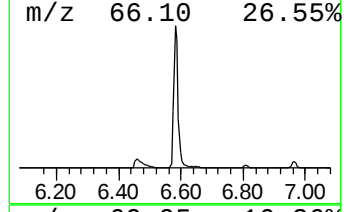
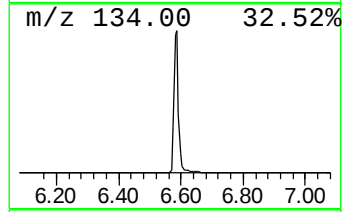
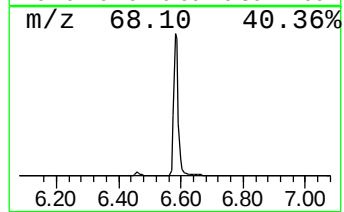
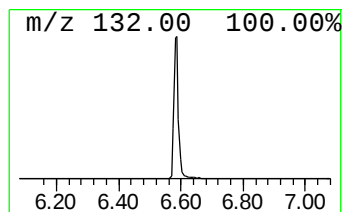
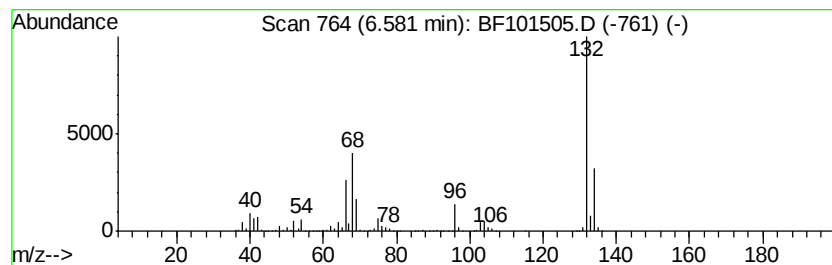
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 unknown6.58 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.58 | 50.58 ng | 1843530 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    |   | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 3    |    |   | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    |   | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 9    |
| 5    |    |   | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

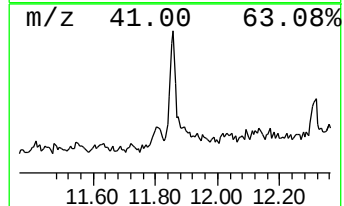
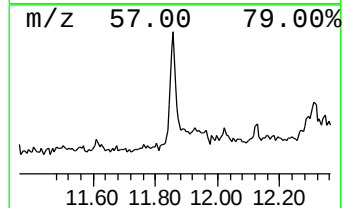
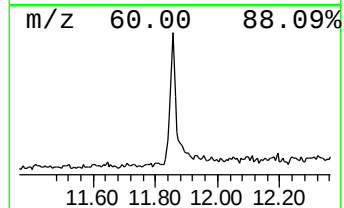
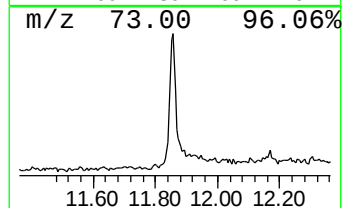
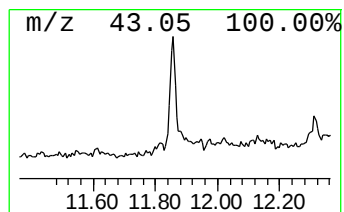
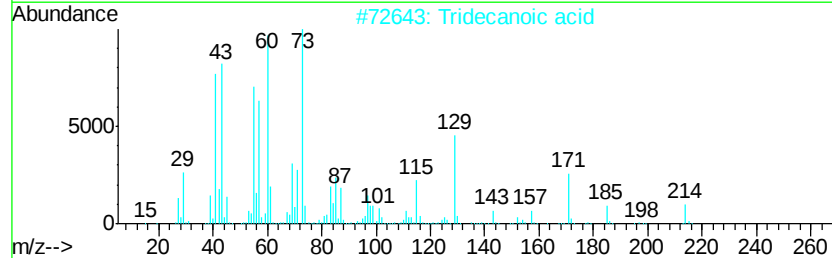
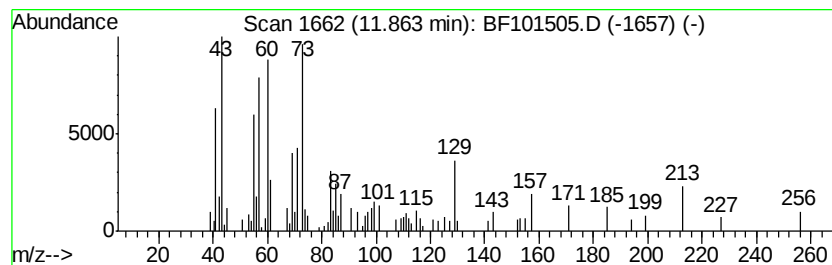
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.86 | 5.35 ng | 182625 | Phenanthrene-d10 | 11.34 |

| 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 | 93   |
| 3       |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 4       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 5       |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 64   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

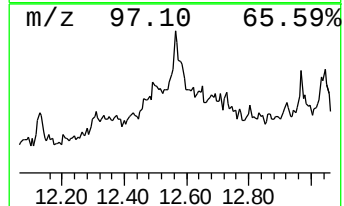
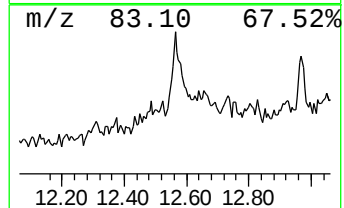
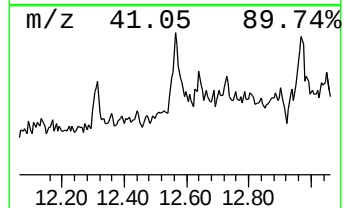
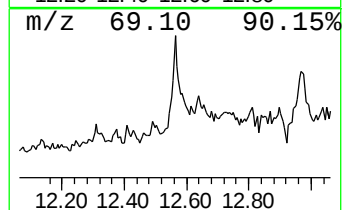
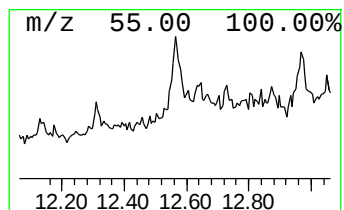
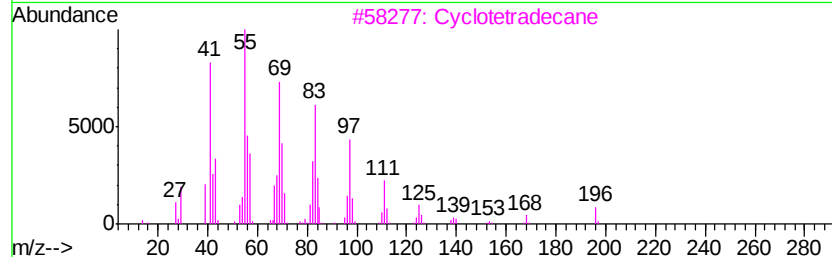
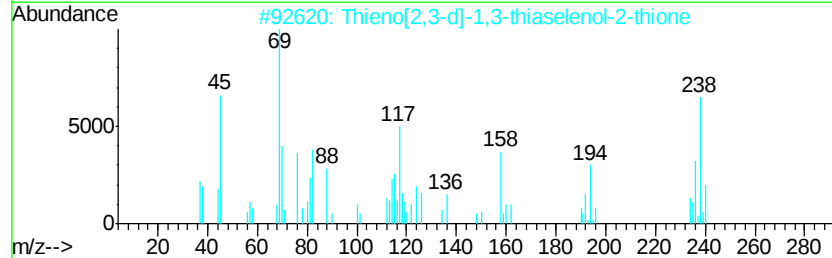
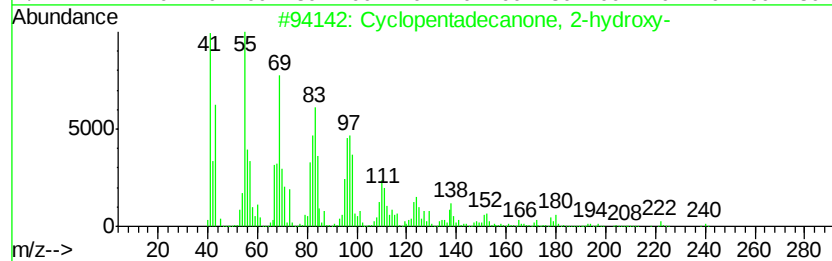
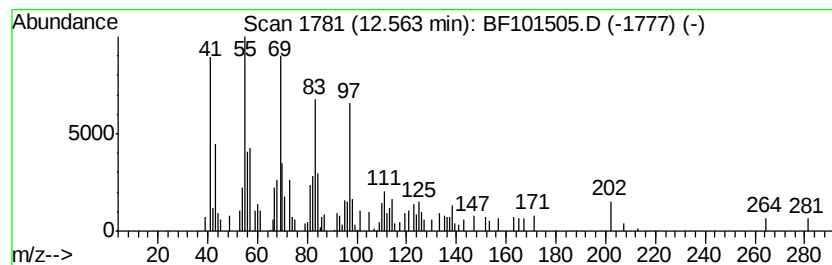
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Cyclopentadecanone, 2-hydroxy- Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.56 | 3.39 ng | 115728 | Phenanthrene-d10 | 11.34 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | Cyclopentadecanone, 2-hydroxy-      | 240 | C15H28O2   | 004727-18-8 | 80   |
| 2    |    | Thieno[2,3-d]-1,3-thiaselenol-2-... | 238 | C5H2S3Se   | 081803-09-0 | 68   |
| 3    |    | Cyclotetradecane                    | 196 | C14H28     | 000295-17-0 | 68   |
| 4    |    | 9-Heptadecanol                      | 256 | C17H36O    | 000624-08-8 | 58   |
| 5    |    | Acetic acid, trifluoro-, undecyl... | 268 | C13H23F3O2 | 053800-01-4 | 58   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

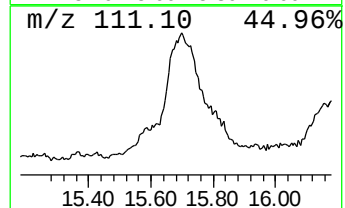
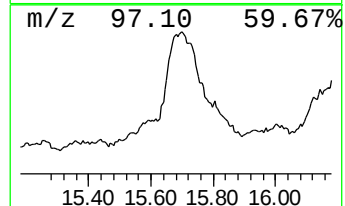
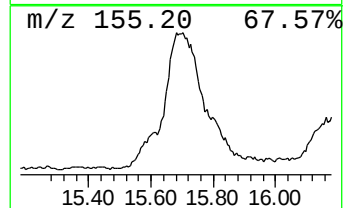
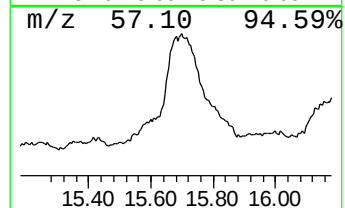
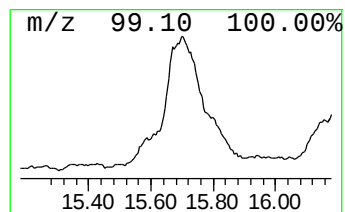
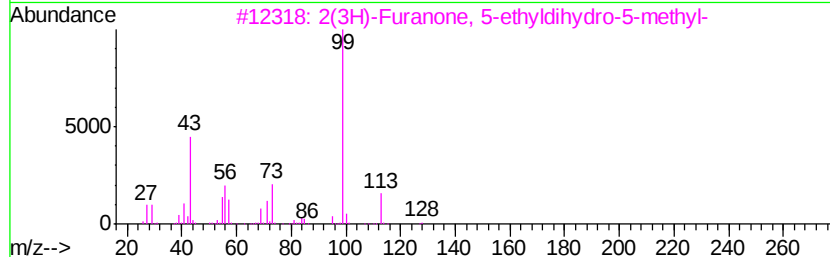
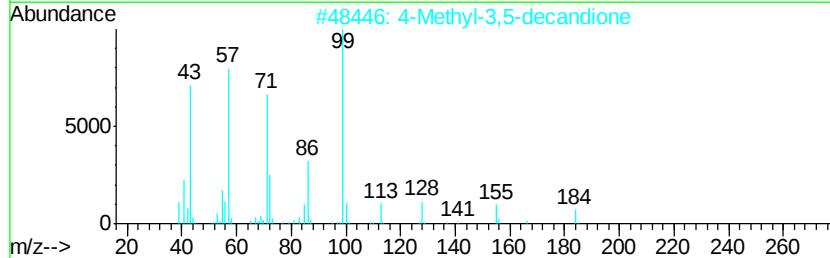
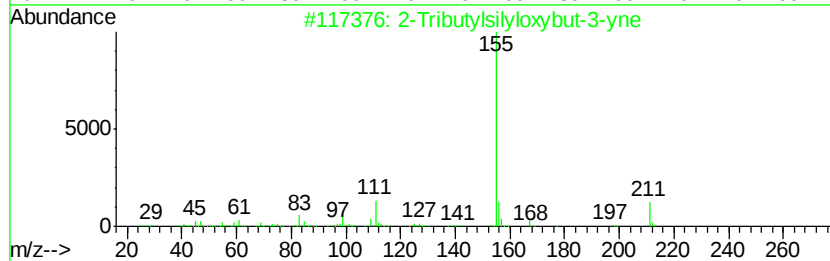
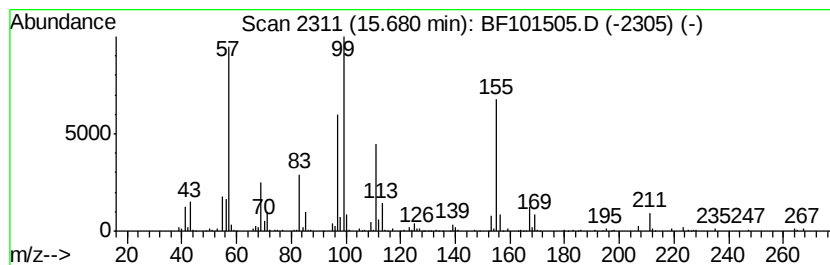
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 unknown15.68 Concentration Rank 3

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 15.68 | 11.91 ng | 386749 | Perylene-d12     | 15.46 |

| Hit# | of | Tentative ID                         | MW  | MolForm   | CAS#         | Qual |
|------|----|--------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 2-Tributylsilyloxybut-3-yne          | 268 | C16H32OSi | 1000299-53-9 | 25   |
| 2    |    | 4-Methyl-3,5-decandione              | 184 | C11H20O2  | 1000374-13-1 | 25   |
| 3    |    | 2(3H)-Furanone, 5-ethylidihydro-5... | 128 | C7H12O2   | 002865-82-9  | 22   |
| 4    |    | 1,4-Dioxaspiro[4.5]decane            | 142 | C8H14O2   | 000177-10-6  | 22   |
| 5    |    | 2-Propylthiazole                     | 127 | C6H9NS    | 017626-75-4  | 18   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF121817\  
Data File : BF101505.D  
Acq On : 19 Dec 2017 3:50  
Operator : SJ/JU  
Sample : I6909-07  
Misc :  
ALS Vial : 32 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
121217-TIDO-E-U-B

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF121417.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 |
| 2-Pentanone, 4-hy... | 5.02  | 3.2     | ng    | 117505   | 1                     | 6.81  | 728974 | 20.0 |
| unknown6.58          | 6.58  | 50.6    | ng    | 1843530  | 1                     | 6.81  | 728974 | 20.0 |
| n-Hexadecanoic acid  | 11.86 | 5.3     | ng    | 182625   | 4                     | 11.34 | 682959 | 20.0 |
| Cyclopentadecanon... | 12.56 | 3.4     | ng    | 115728   | 4                     | 11.34 | 682959 | 20.0 |
| unknown15.68         | 15.68 | 11.9    | ng    | 386749   | 6                     | 15.46 | 649616 | 20.0 |