

Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\  
 Data File : BF095970.D  
 Acq On : 16 Jun 2017 22:59  
 Operator : SJ/MA  
 Sample : I3681-01  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RO-272031-72-11978-COMP

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-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         | 4.522       | 495           | 499         | 517          | rBV2     | 51984          | 160313        | 7.80%           | 1.019%        |
| 2         | 5.216       | 614           | 617         | 654          | rBV      | 786497         | 1652530       | 80.35%          | 10.504%       |
| 3         | 6.898       | 898           | 903         | 913          | rBV      | 997291         | 1555999       | 75.66%          | 9.891%        |
| 4         | 6.981       | 913           | 917         | 937          | rVB      | 1240880        | 1956786       | 95.15%          | 12.438%       |
| 5         | 7.322       | 971           | 975         | 991          | rVB      | 302157         | 416623        | 20.26%          | 2.648%        |
| 6         | 7.557       | 1010          | 1015        | 1034         | rBV      | 1035962        | 1373943       | 66.81%          | 8.734%        |
| 7         | 8.239       | 1127          | 1131        | 1151         | rBV      | 678675         | 1023732       | 49.78%          | 6.507%        |
| 8         | 9.351       | 1316          | 1320        | 1340         | rBV      | 407357         | 566115        | 27.53%          | 3.599%        |
| 9         | 11.133      | 1617          | 1623        | 1637         | rBV      | 1615869        | 2056577       | 100.00%         | 13.073%       |
| 10        | 11.827      | 1737          | 1741        | 1751         | rBV      | 218907         | 295630        | 14.37%          | 1.879%        |
| 11        | 12.168      | 1795          | 1799        | 1805         | rBV2     | 476653         | 597356        | 29.05%          | 3.797%        |
| 12        | 12.215      | 1805          | 1807        | 1814         | rVB2     | 18419          | 21932         | 1.07%           | 0.139%        |
| 13        | 13.027      | 1940          | 1945        | 1951         | rVB      | 23587          | 27900         | 1.36%           | 0.177%        |
| 14        | 13.468      | 2015          | 2020        | 2035         | rBV      | 643943         | 973267        | 47.32%          | 6.187%        |
| 15        | 13.798      | 2071          | 2076        | 2084         | rVB      | 23925          | 32859         | 1.60%           | 0.209%        |
| 16        | 14.562      | 2202          | 2206        | 2223         | rVB      | 365912         | 511220        | 24.86%          | 3.250%        |
| 17        | 15.586      | 2376          | 2380        | 2395         | rBV2     | 60438          | 88735         | 4.31%           | 0.564%        |
| 18        | 16.692      | 2564          | 2568        | 2581         | rBV3     | 28524          | 49424         | 2.40%           | 0.314%        |
| 19        | 16.939      | 2605          | 2610        | 2617         | rVB      | 1156419        | 1354714       | 65.87%          | 8.611%        |
| 20        | 18.203      | 2820          | 2825        | 2835         | rBV2     | 41234          | 78837         | 3.83%           | 0.501%        |
| 21        | 18.286      | 2835          | 2839        | 2849         | rVV      | 295154         | 400124        | 19.46%          | 2.543%        |
| 22        | 19.956      | 3119          | 3123        | 3133         | rBV      | 306871         | 414444        | 20.15%          | 2.634%        |
| 23        | 20.468      | 3200          | 3210        | 3216         | rBV      | 27831          | 71841         | 3.49%           | 0.457%        |
| 24        | 20.785      | 3261          | 3264        | 3267         | rVB5     | 17577          | 23739         | 1.15%           | 0.151%        |
| 25        | 21.650      | 3407          | 3411        | 3420         | rVB8     | 12671          | 27164         | 1.32%           | 0.173%        |

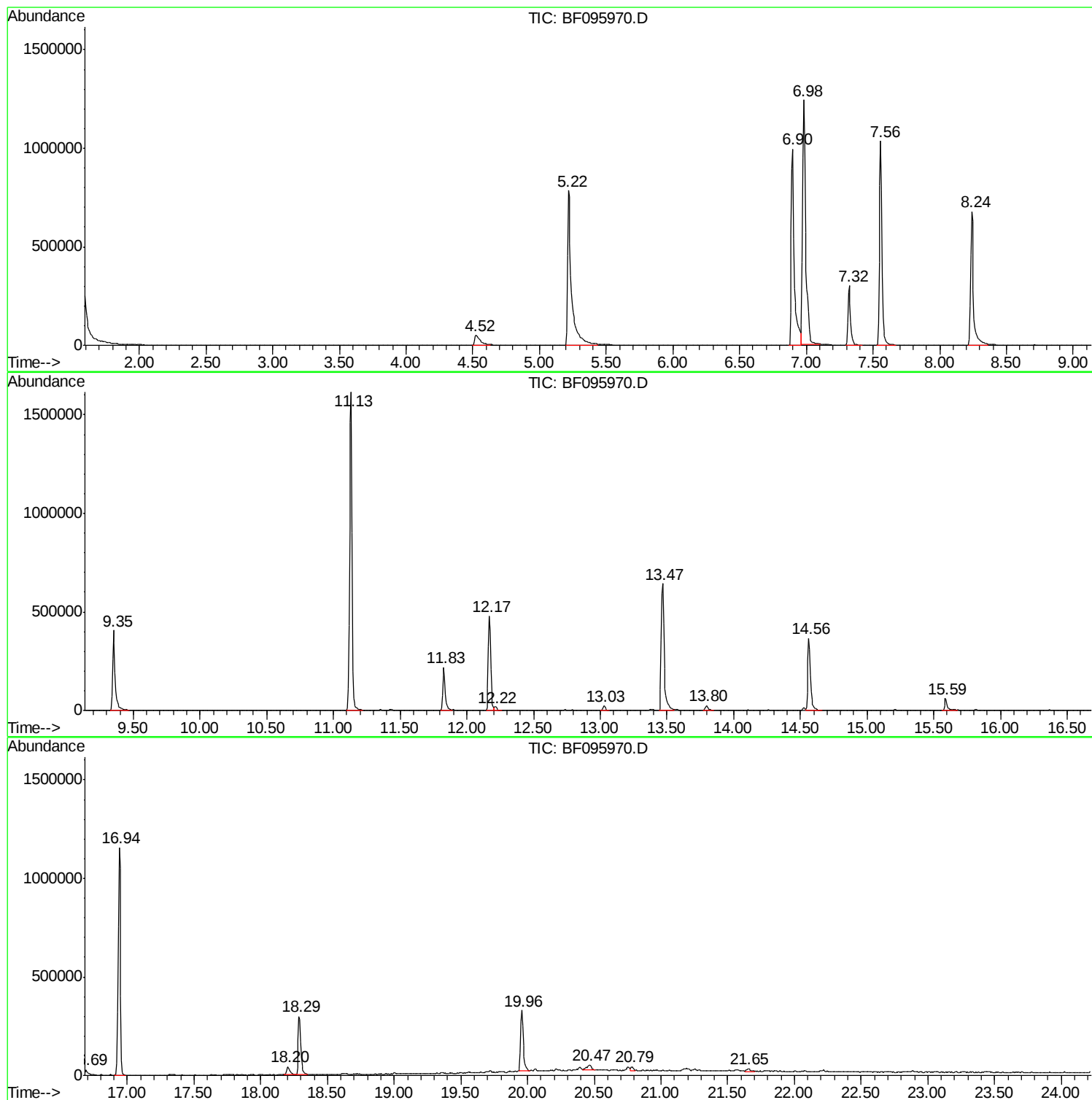
Sum of corrected areas: 15731804

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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

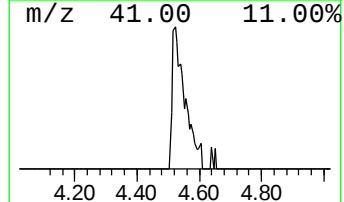
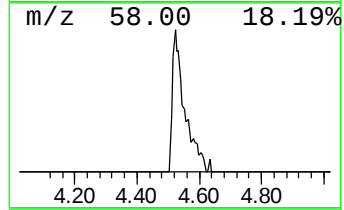
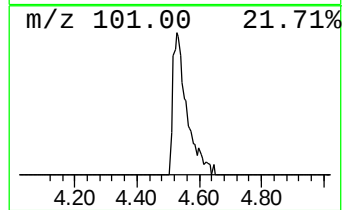
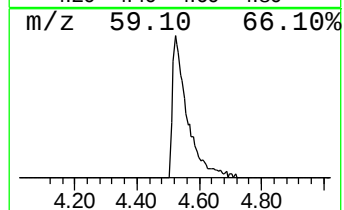
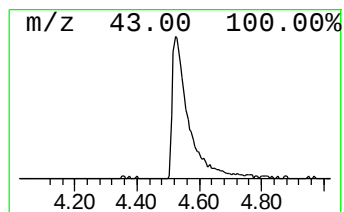
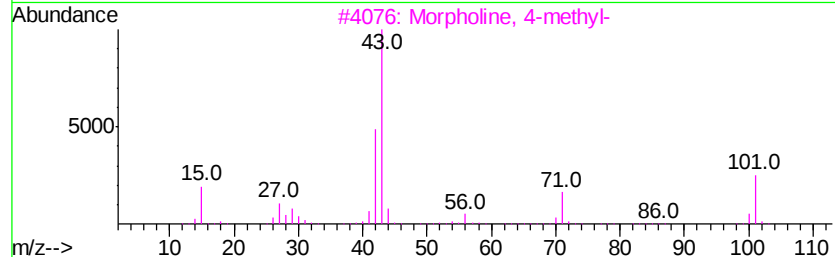
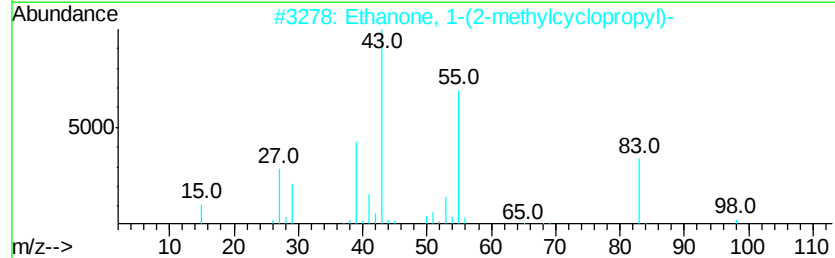
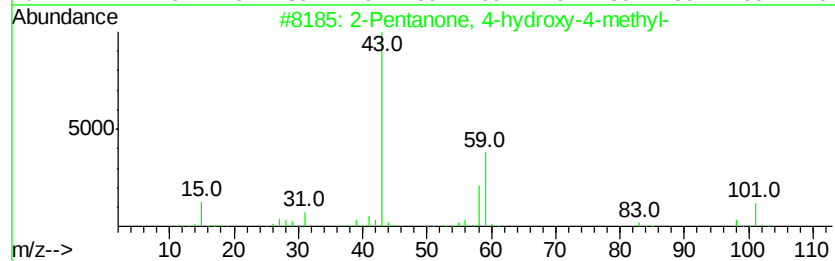
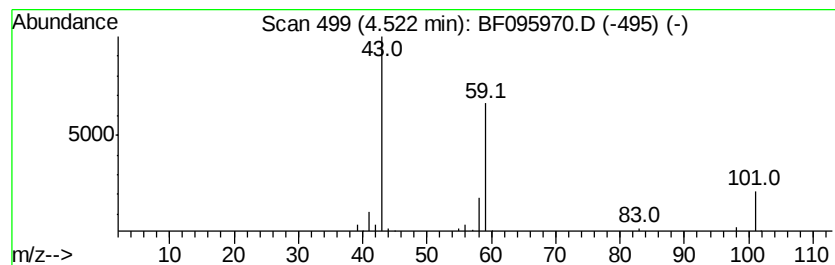
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.52 | 7.70 ng | 160313 | 1,4-Dichlorobenzene-d4 | 7.32 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 50   |
| 2    |    | Ethanone, 1-(2-methylcyclopropyl)- | 98  | C6H10O  | 000930-56-3 | 9    |
| 3    |    | Morpholine, 4-methyl-              | 101 | C5H11NO | 000109-02-4 | 9    |
| 4    |    | Propanamide, N-ethyl-              | 101 | C5H11NO | 005129-72-6 | 9    |
| 5    |    | (+)-4-Amino-4,5-dihydro-2(3H)-f... | 101 | C4H7NO2 | 016504-58-8 | 9    |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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

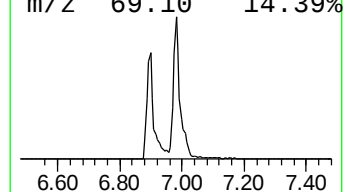
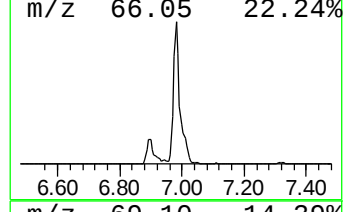
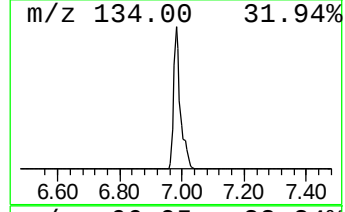
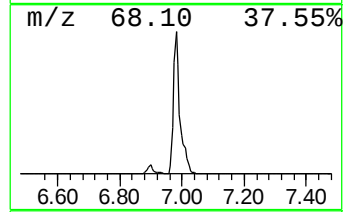
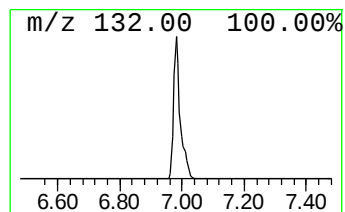
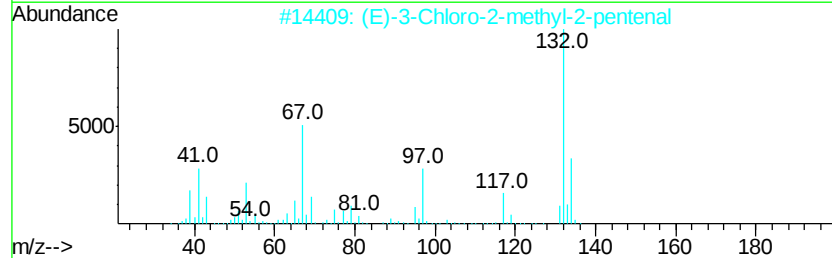
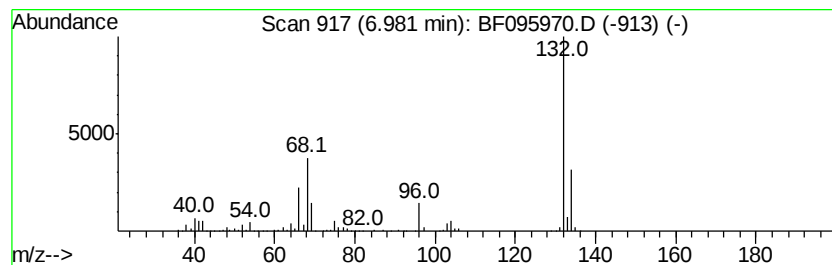
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown6.98 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.98 | 93.94 ng | 1956790 | 1,4-Dichlorobenzene-d4 | 7.32 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 25   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 25   |
| 3    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 12   |
| 4    |    | 4-Methylpyrrolo[1,2-a]pyrazine   | 132 | C8H8N2    | 064608-60-2  | 9    |
| 5    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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

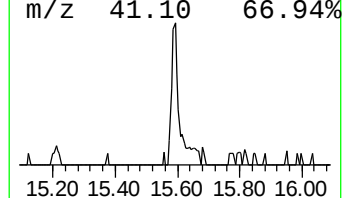
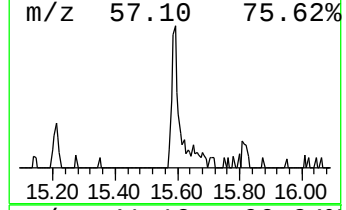
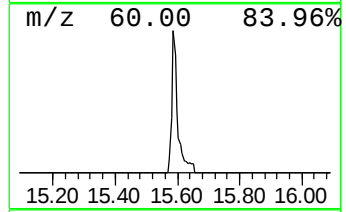
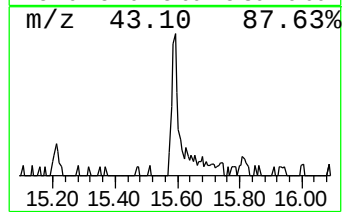
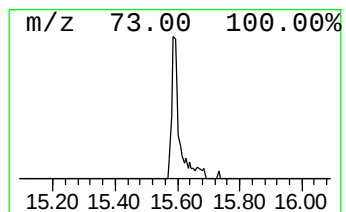
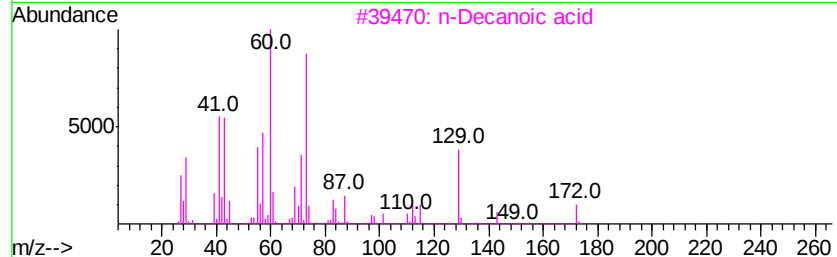
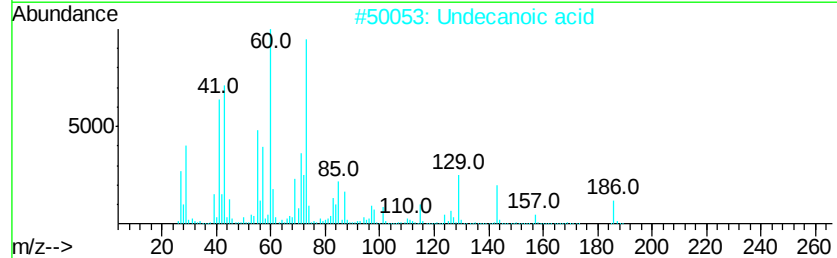
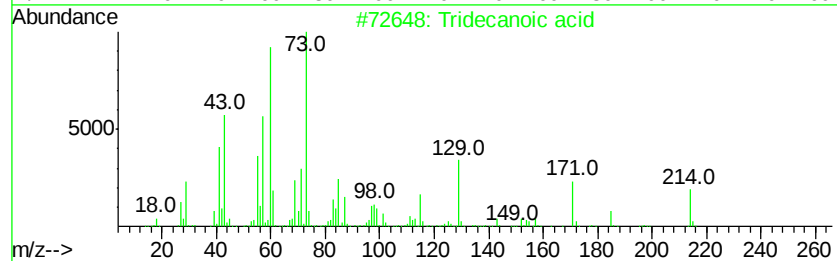
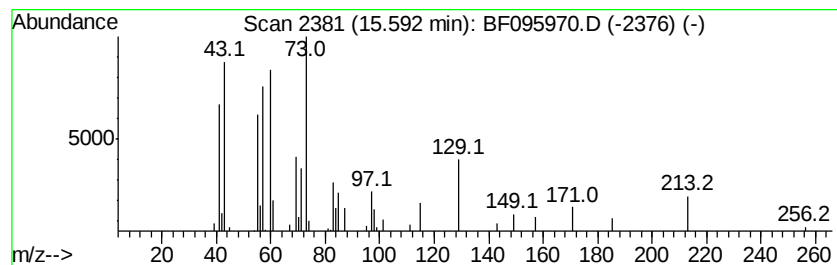
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Tridecanoic acid Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 15.59 | 3.47 ng | 88735 | Phenanthrene-d10 | 14.56 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|---------|---|-------------------------------------|-----|----------|--------------|------|
| 1       |   | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9  | 80   |
| 2       |   | Undecanoic acid                     | 186 | C11H22O2 | 000112-37-8  | 64   |
| 3       |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5  | 58   |
| 4       |   | Oxalic acid, cyclobutyl dodecyl ... | 312 | C18H32O4 | 1000309-70-3 | 22   |
| 5       |   | Oxalic acid, allyl hexadecyl ester  | 354 | C21H38O4 | 1000309-24-4 | 14   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

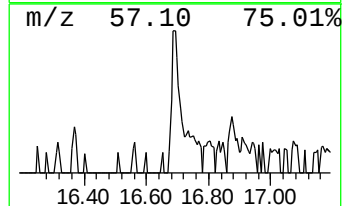
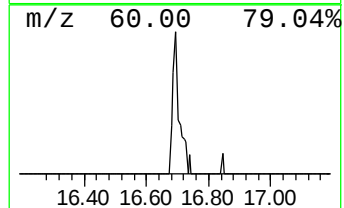
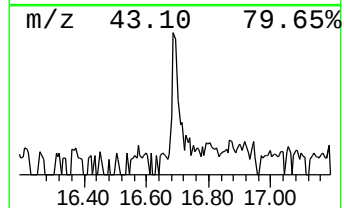
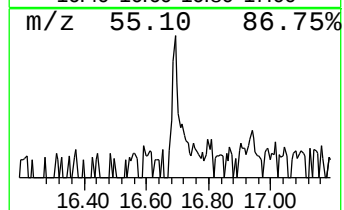
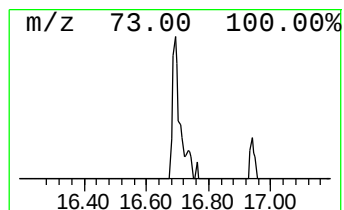
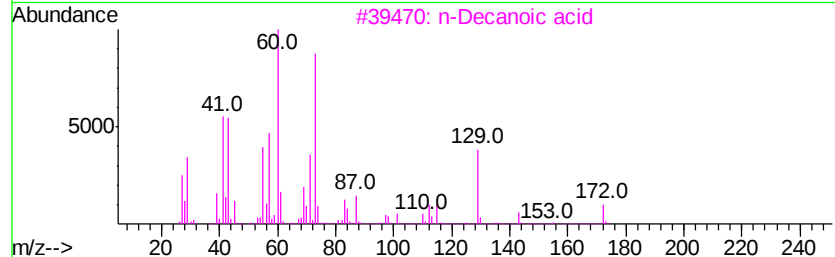
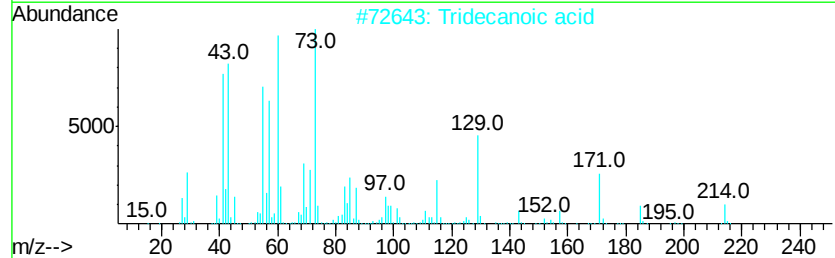
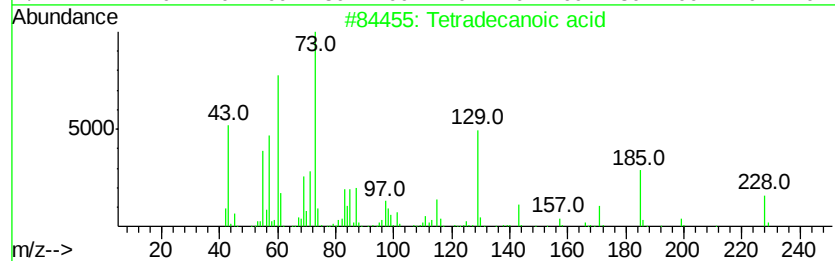
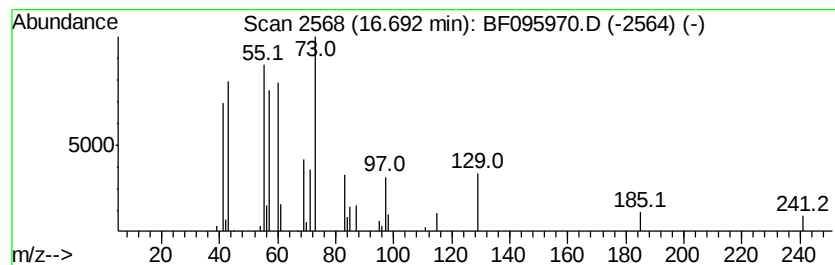
Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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 5 Tetradecanoic acid Concentration Rank 7

| R.T.      | EstConc                             | Area  | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|-------|------------------|--------------|------|
| 16.69     | 2.47 ng                             | 49424 | Chrysene-d12     | 18.29        |      |
| Hit# of 5 | Tentative ID                        | MW    | MolForm          | CAS#         | Qual |
| 1         | Tetradecanoic acid                  | 228   | C14H28O2         | 000544-63-8  | 72   |
| 2         | Tridecanoic acid                    | 214   | C13H26O2         | 000638-53-9  | 64   |
| 3         | n-Decanoic acid                     | 172   | C10H20O2         | 000334-48-5  | 59   |
| 4         | Hexatriacontyl pentafluoropropio... | 669   | C39H73F5O2       | 1000351-89-0 | 14   |
| 5         | Oxalic acid, allyl tetradecyl ester | 326   | C19H34O4         | 1000309-24-2 | 14   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

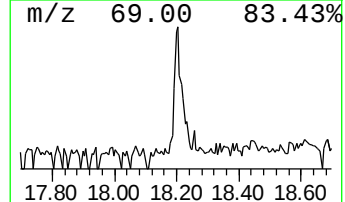
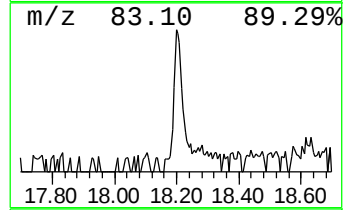
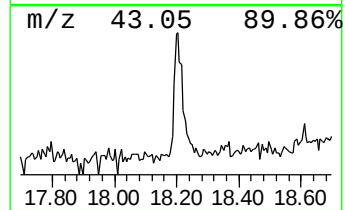
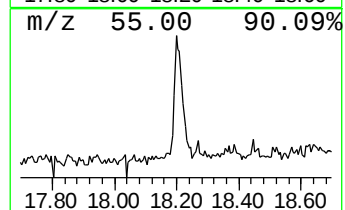
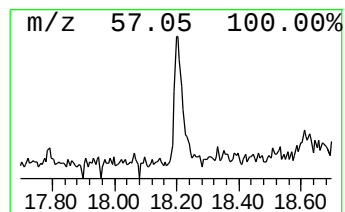
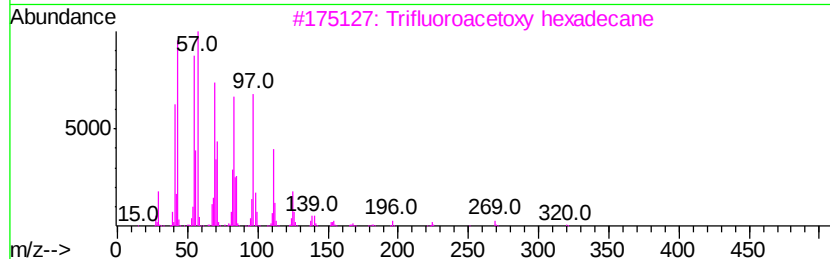
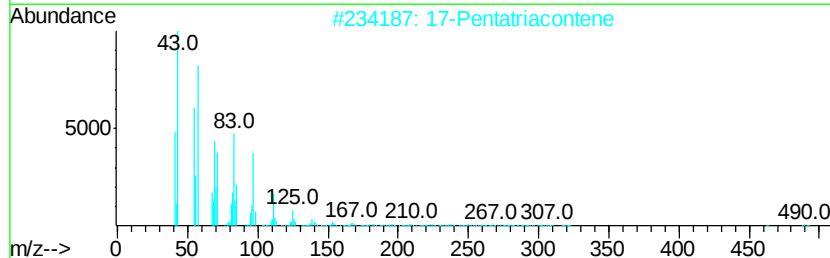
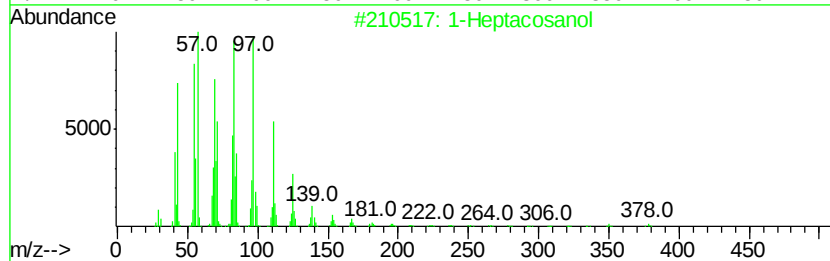
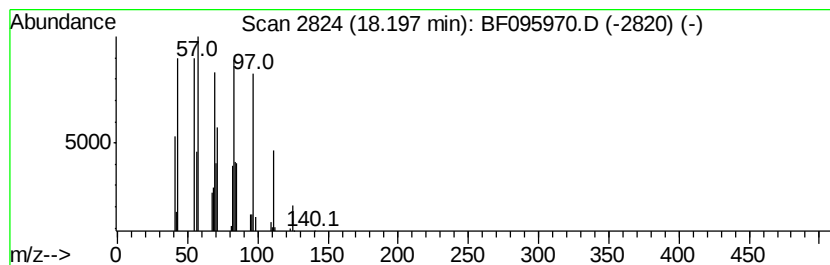
Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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 1-Heptacosanol Concentration Rank 4

| R.T.      | EstConc                     | Area  | Relative to ISTD | R.T.        |      |
|-----------|-----------------------------|-------|------------------|-------------|------|
| 18.20     | 3.94 ng                     | 78837 | Chrysene-d12     | 18.29       |      |
| Hit# of 5 | Tentative ID                | MW    | MolForm          | CAS#        | Qual |
| 1         | 1-Heptacosanol              | 396   | C27H56O          | 002004-39-9 | 94   |
| 2         | 17-Pentatriacontene         | 491   | C35H70           | 006971-40-0 | 91   |
| 3         | Trifluoroacetoxv hexadecane | 338   | C18H33F3O2       | 006222-03-3 | 91   |
| 4         | 1-Heneicosanol              | 312   | C21H44O          | 015594-90-8 | 87   |
| 5         | Behenic alcohol             | 326   | C22H46O          | 000661-19-8 | 87   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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

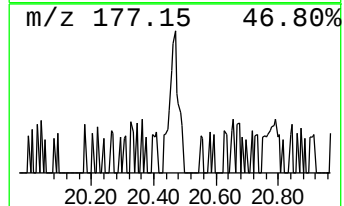
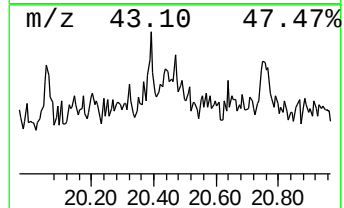
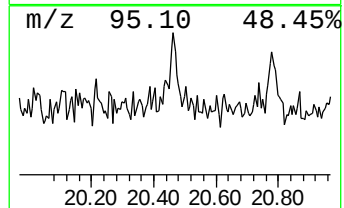
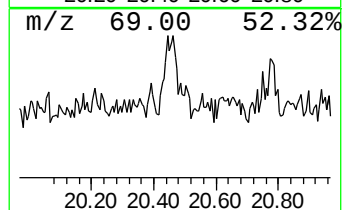
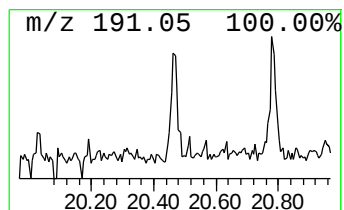
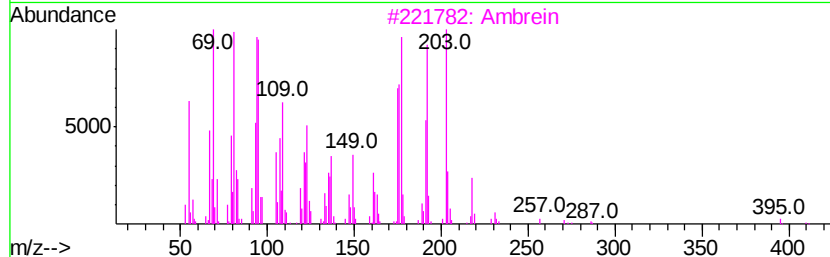
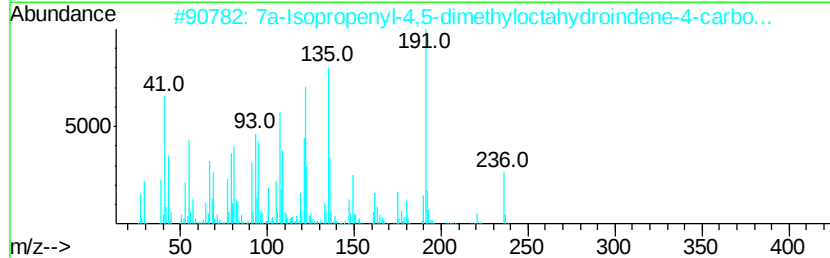
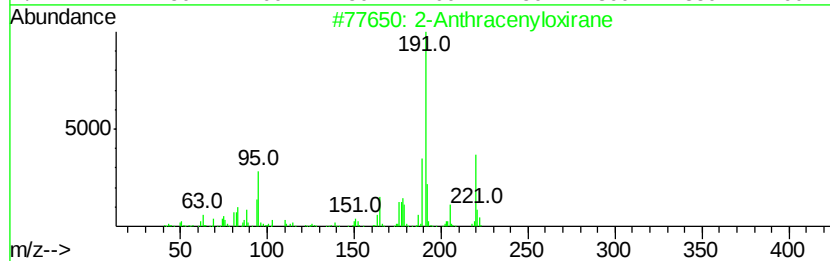
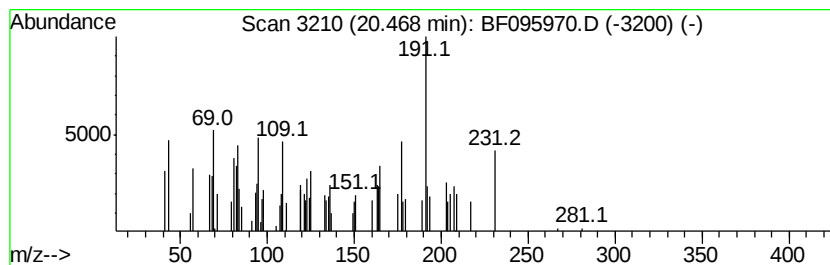
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 unknown20.47 Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 20.47 | 3.47 ng | 71841 | Perylene-d12     | 19.96 |

| Hit# | of                                  | Tentative ID                     | MW  | MolForm  | CAS#         | Qual |
|------|-------------------------------------|----------------------------------|-----|----------|--------------|------|
| 1    | 2                                   | Anthracenyloxirane               | 220 | C16H12O  | 052643-86-4  | 16   |
| 2    | 7a                                  | Isopropenyl-4,5-dimethyloctah... | 236 | C15H24O2 | 1000192-14-7 | 12   |
| 3    | Ambrein                             |                                  | 428 | C30H52O  | 1000292-95-3 | 11   |
| 4    | Silane, 1,3-decadiynyltrimethyl-    |                                  | 206 | C13H22Si | 084751-17-7  | 10   |
| 5    | Pyrido[3,4-d]pyrimidine-2,4(1H,3... |                                  | 191 | C9H9N3O2 | 022389-83-9  | 10   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF061617\  
Data File : BF095970.D  
Acq On : 16 Jun 2017 22:59  
Operator : SJ/MA  
Sample : I3681-01  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RO-272031-72-11978-COMP

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 |
| 2-Pentanone, 4-hy... | 4.52  | 7.7     | ng    | 160313   | 1                       | 7.32  | 416623 | 20.0 |
| unknown6.98          | 6.98  | 93.9    | ng    | 1956790  | 1                       | 7.32  | 416623 | 20.0 |
| Tridecanoic acid     | 15.59 | 3.5     | ng    | 88735    | 4                       | 14.56 | 511220 | 20.0 |
| Tetradecanoic acid   | 16.69 | 2.5     | ng    | 49424    | 5                       | 18.29 | 400124 | 20.0 |
| 1-Heptacosanol       | 18.20 | 3.9     | ng    | 78837    | 5                       | 18.29 | 400124 | 20.0 |
| unknown20.47         | 20.47 | 3.5     | ng    | 71841    | 6                       | 19.96 | 414444 | 20.0 |