

Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF121919\  
 Data File : BF118282.D  
 Acq On : 19 Dec 2019 16:30  
 Operator : JU  
 Sample : PB125606BL  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB125606BL

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

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

Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120619.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         | 5.087       | 505           | 510         | 525          | rBV      | 427624         | 577561        | 11.73%          | 1.725%        |
| 2         | 5.487       | 574           | 578         | 581          | rBV      | 3068454        | 3019542       | 61.33%          | 9.017%        |
| 3         | 6.493       | 744           | 749         | 752          | rBV      | 2995756        | 3173295       | 64.45%          | 9.476%        |
| 4         | 6.628       | 768           | 772         | 776          | rBV      | 3467443        | 3494078       | 70.97%          | 10.434%       |
| 5         | 6.857       | 807           | 811         | 824          | rVB      | 805161         | 673556        | 13.68%          | 2.011%        |
| 6         | 7.016       | 833           | 838         | 841          | rBV      | 3213266        | 2752518       | 55.91%          | 8.220%        |
| 7         | 7.422       | 902           | 907         | 923          | rBV      | 1822408        | 2074408       | 42.13%          | 6.195%        |
| 8         | 8.145       | 1025          | 1030        | 1043         | rBV      | 844613         | 868604        | 17.64%          | 2.594%        |
| 9         | 9.222       | 1208          | 1213        | 1228         | rBV      | 4056486        | 4316479       | 87.67%          | 12.890%       |
| 10        | 9.904       | 1324          | 1329        | 1342         | rVB      | 1079450        | 1048546       | 21.30%          | 3.131%        |
| 11        | 10.704      | 1460          | 1465        | 1488         | rBV      | 2842828        | 2970316       | 60.33%          | 8.870%        |
| 12        | 11.398      | 1580          | 1583        | 1592         | rBV      | 1113481        | 1091986       | 22.18%          | 3.261%        |
| 13        | 12.992      | 1849          | 1854        | 1857         | rBV      | 4841309        | 4923529       | 100.00%         | 14.703%       |
| 14        | 14.051      | 2030          | 2034        | 2044         | rBV      | 806907         | 886271        | 18.00%          | 2.647%        |
| 15        | 14.510      | 2103          | 2112        | 2115         | rBV      | 83827          | 85414         | 1.73%           | 0.255%        |
| 16        | 14.821      | 2158          | 2165        | 2172         | rBV      | 119230         | 144838        | 2.94%           | 0.433%        |
| 17        | 15.163      | 2217          | 2223        | 2229         | rBV      | 144654         | 168314        | 3.42%           | 0.503%        |
| 18        | 15.545      | 2282          | 2288        | 2304         | rBV2     | 533791         | 850037        | 17.26%          | 2.538%        |
| 19        | 15.992      | 2357          | 2364        | 2374         | rBV      | 115038         | 191394        | 3.89%           | 0.572%        |
| 20        | 16.510      | 2444          | 2452        | 2460         | rBV2     | 64146          | 125186        | 2.54%           | 0.374%        |
| 21        | 17.115      | 2547          | 2555        | 2563         | rBV5     | 22723          | 51364         | 1.04%           | 0.153%        |

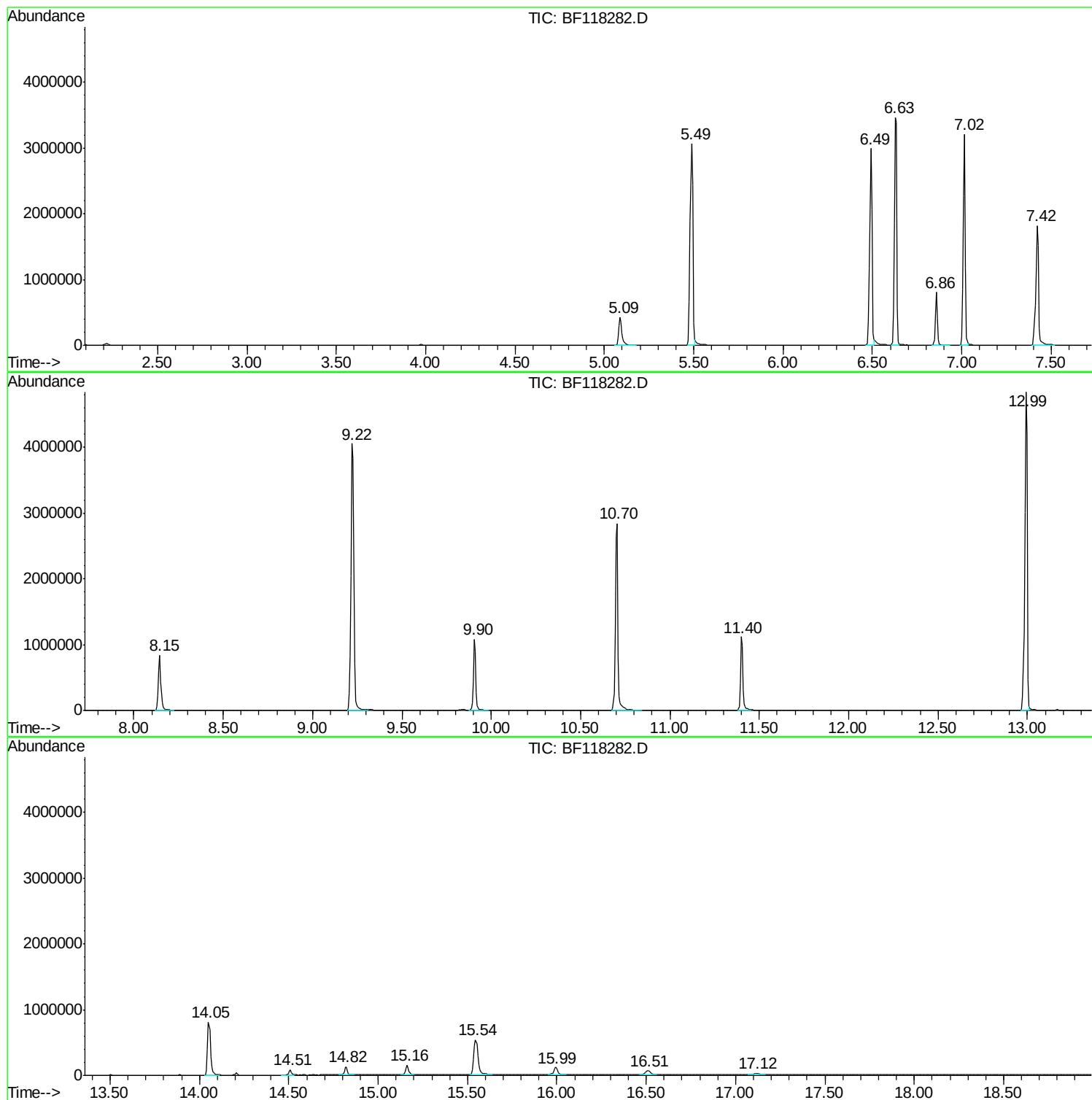
Sum of corrected areas: 33487236

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

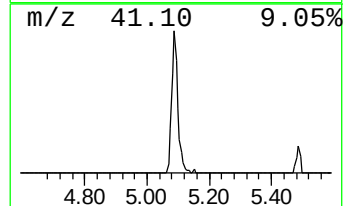
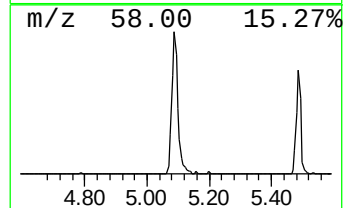
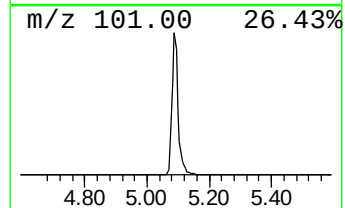
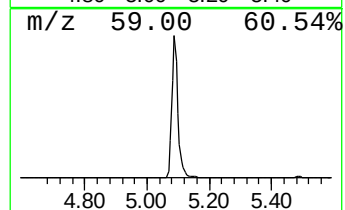
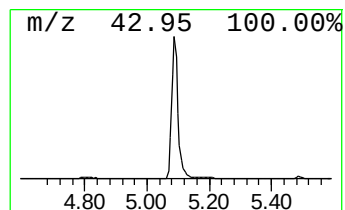
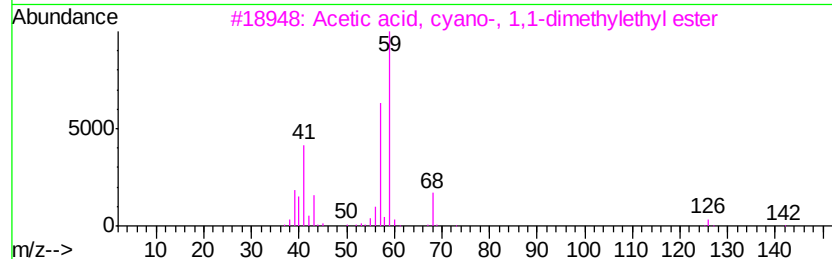
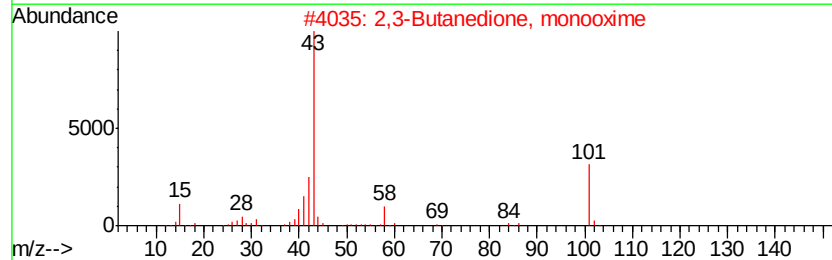
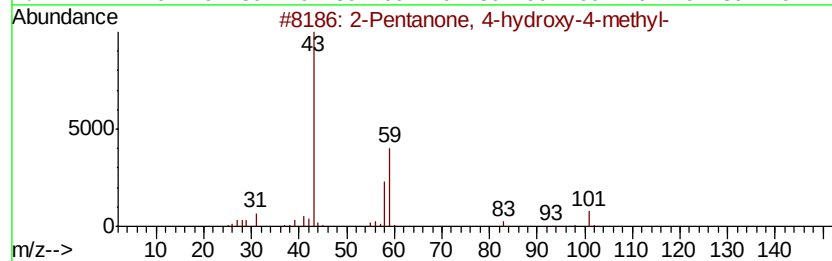
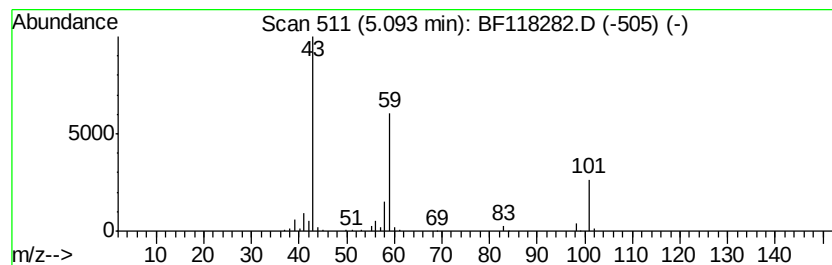
Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.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.      |
|---------|--------------------------------------|--------------|------------------------|-----------|
| 5.09    | 17.15 ng                             | 577561       | 1,4-Dichlorobenzene-d4 | 6.86      |
| Hit# of | 5                                    | Tentative ID | MW MolForm             | CAS# Qual |
| 1       | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 C6H12O2  | 000123-42-2            | 56        |
| 2       | 2,3-Butanedione, monooxime           | 101 C4H7NO2  | 000057-71-6            | 25        |
| 3       | Acetic acid, cyano-, 1,1-dimethyl... | 141 C7H11NO2 | 001116-98-9            | 17        |
| 4       | Acetone                              | 58 C3H6O     | 000067-64-1            | 10        |
| 5       | (+)-4-Amino-4,5-dihydro-2(3H)-f...   | 101 C4H7NO2  | 016504-58-8            | 9         |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

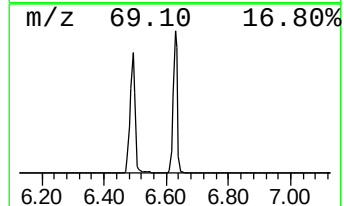
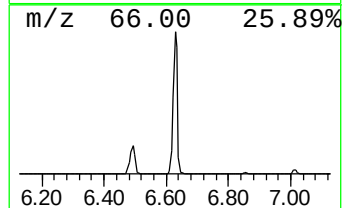
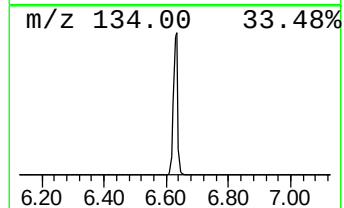
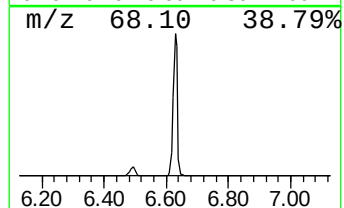
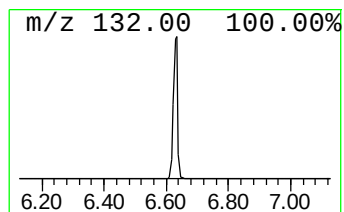
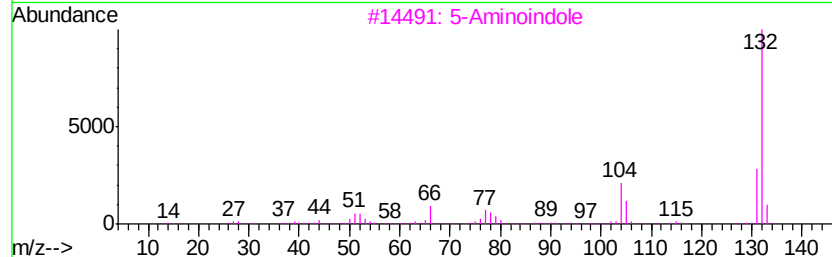
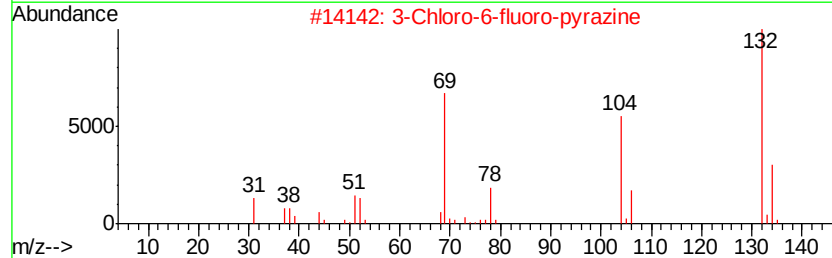
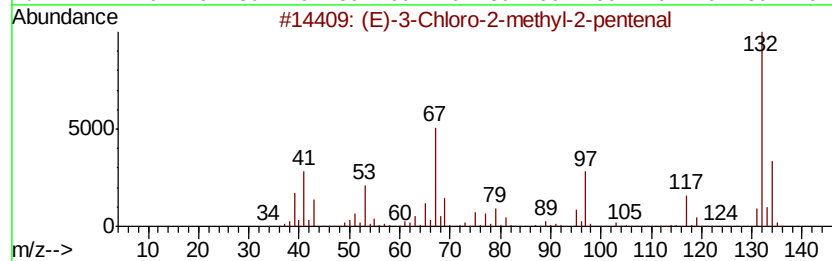
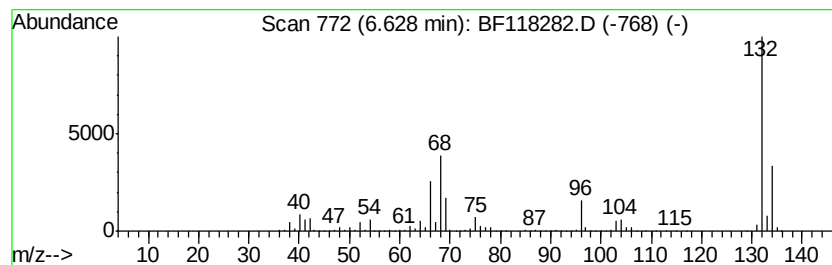
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown6.63 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 6.63 | 103.75 ng | 3494080 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 16   |
| 3    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
 Data File : BF118282.D  
 Acq On : 19 Dec 2019 16:30  
 Operator : JU  
 Sample : PB125606BL  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

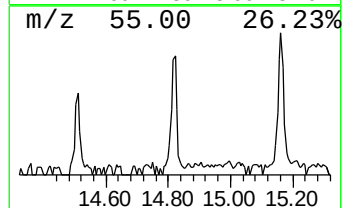
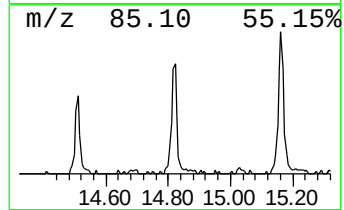
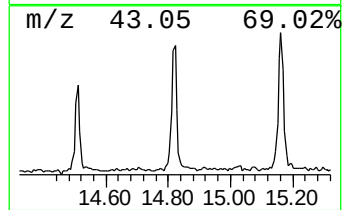
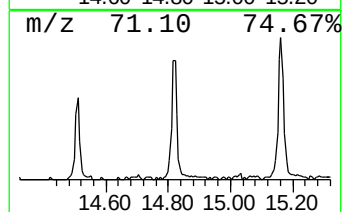
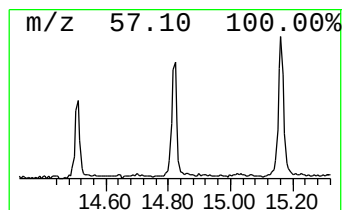
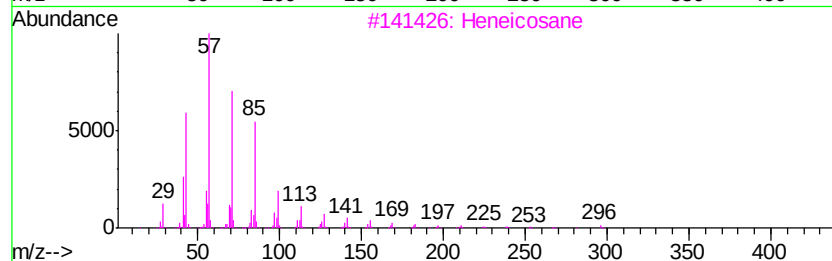
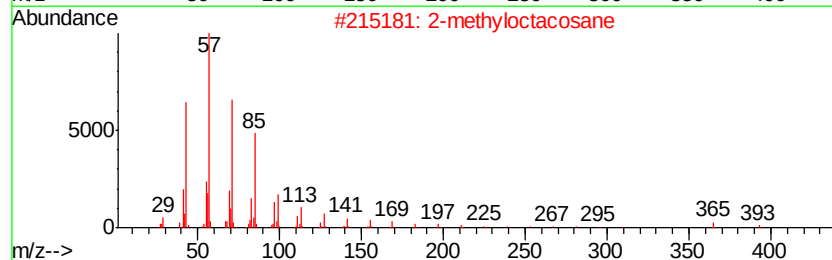
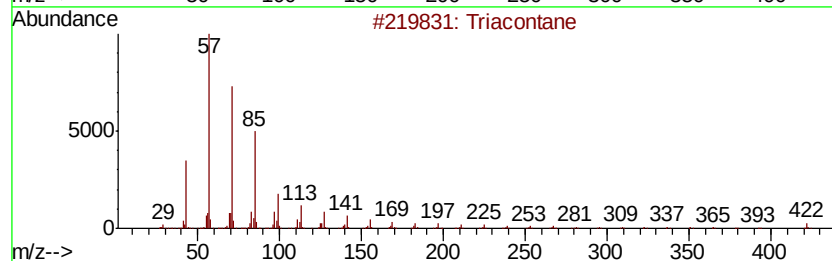
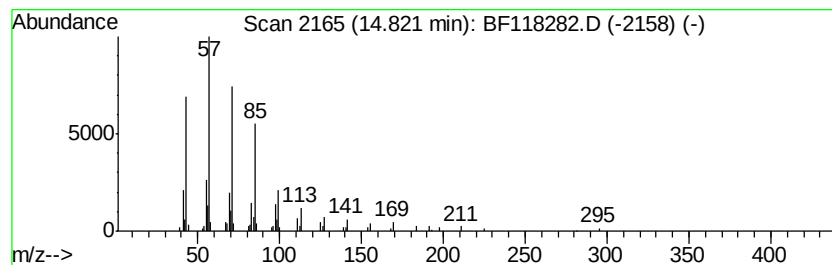
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
 Peak Number 4 Triacontane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.82 | 3.41 ng | 144838 | Perylene-d12     | 15.54 |

| Hit# of 5 | Tentative ID       | MW  | MolForm | CAS#         | Qual |
|-----------|--------------------|-----|---------|--------------|------|
| 1         | Triacontane        | 422 | C30H62  | 000638-68-6  | 91   |
| 2         | 2-methyloctacosane | 408 | C29H60  | 1000376-72-8 | 91   |
| 3         | Heneicosane        | 296 | C21H44  | 000629-94-7  | 91   |
| 4         | Tetratetracontane  | 619 | C44H90  | 007098-22-8  | 90   |
| 5         | Docosane           | 310 | C22H46  | 000629-97-0  | 87   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

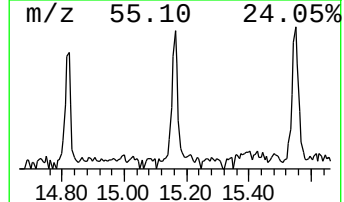
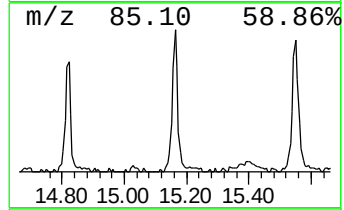
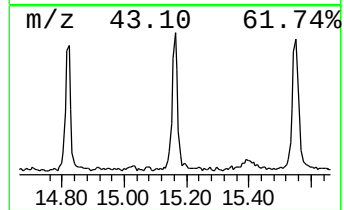
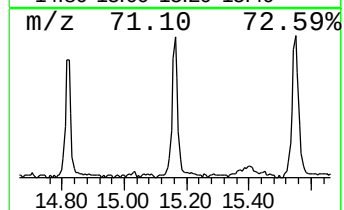
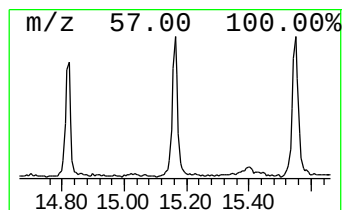
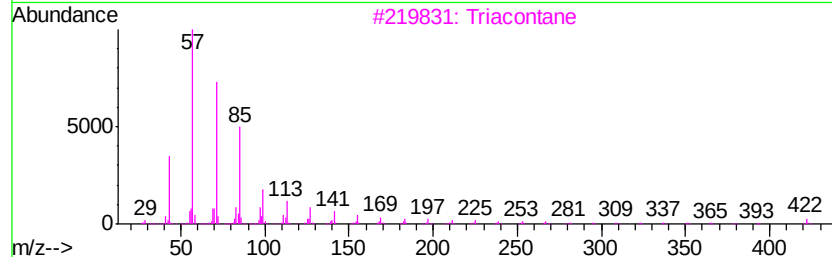
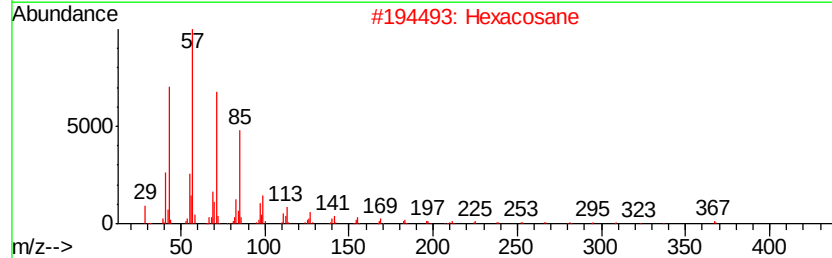
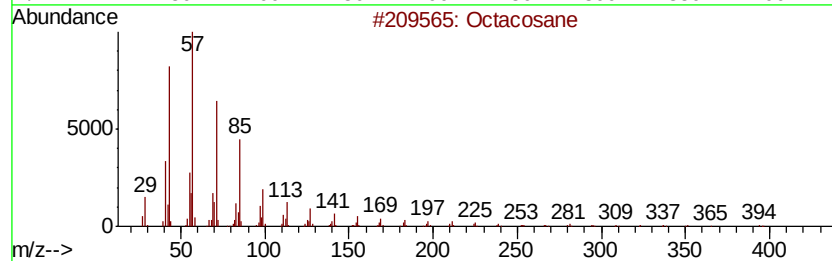
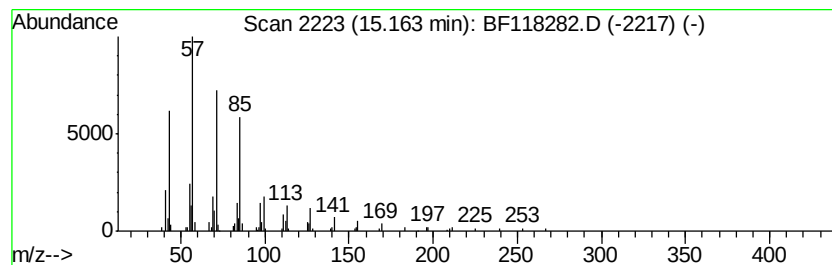
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Octacosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.16 | 3.96 ng | 168314 | Perylene-d12     | 15.54 |

| Hit# of | 5                     | Tentative ID | MW  | MolForm | CAS#         | Qual |
|---------|-----------------------|--------------|-----|---------|--------------|------|
| 1       | Octacosane            |              | 394 | C28H58  | 000630-02-4  | 91   |
| 2       | Hexacosane            |              | 366 | C26H54  | 000630-01-3  | 91   |
| 3       | triacontane           |              | 422 | C30H62  | 000638-68-6  | 91   |
| 4       | 2-methyloctacosane    |              | 408 | C29H60  | 1000376-72-8 | 91   |
| 5       | Heptadecane, 9-octyl- |              | 352 | C25H52  | 007225-64-1  | 91   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

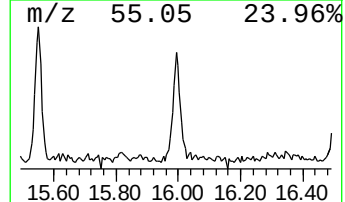
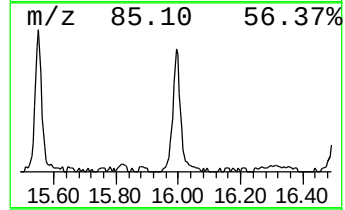
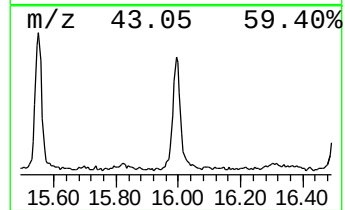
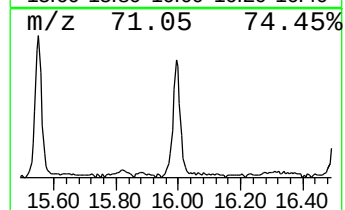
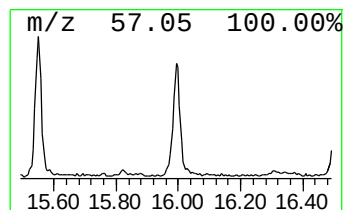
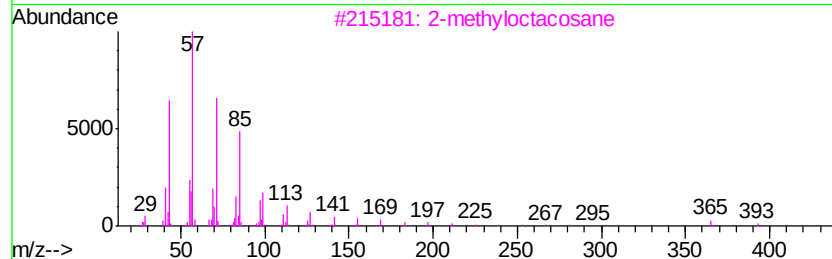
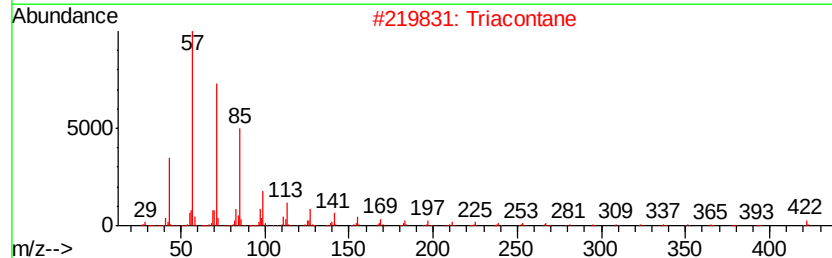
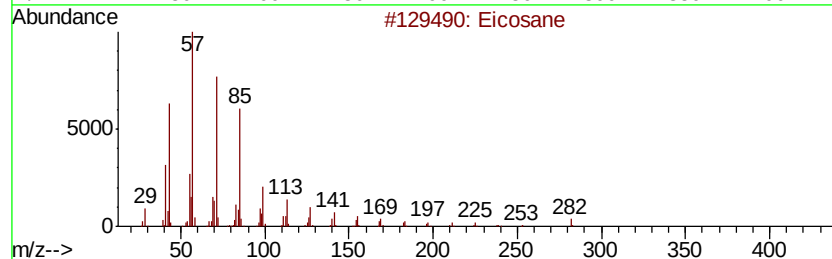
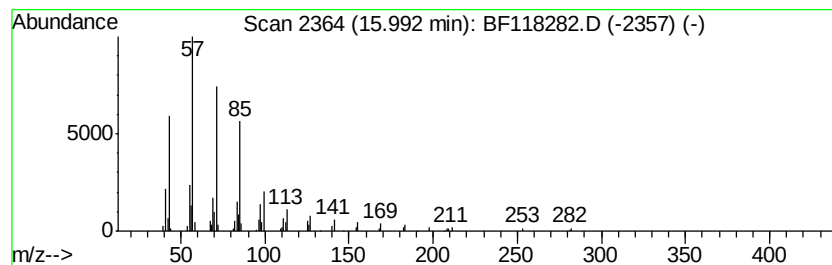
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 6 Eicosane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.99 | 4.50 ng | 191394 | Perylene-d12     | 15.54 |

| Hit# | of | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|------|----|-----------------------|-----|---------|--------------|------|
| 1    | 5  | Eicosane              | 282 | C20H42  | 000112-95-8  | 96   |
| 2    |    | Triacontane           | 422 | C30H62  | 000638-68-6  | 91   |
| 3    |    | 2-methyloctacosane    | 408 | C29H60  | 1000376-72-8 | 91   |
| 4    |    | Heneicosane           | 296 | C21H44  | 000629-94-7  | 91   |
| 5    |    | Heptadecane, 9-octyl- | 352 | C25H52  | 007225-64-1  | 91   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF120619.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

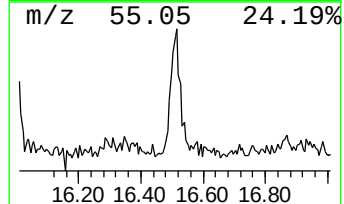
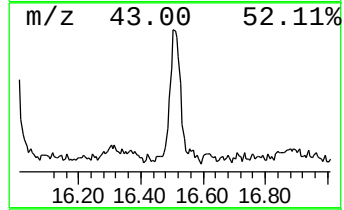
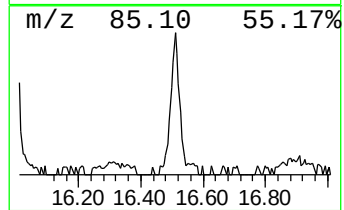
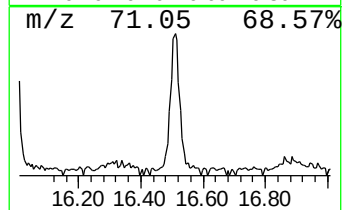
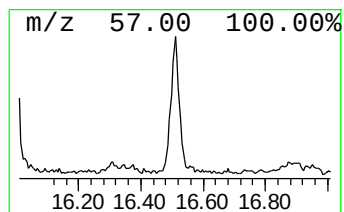
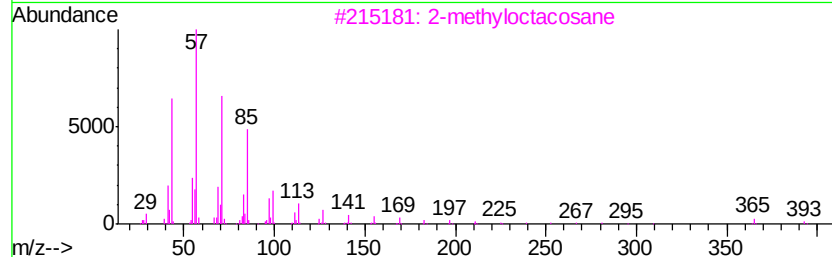
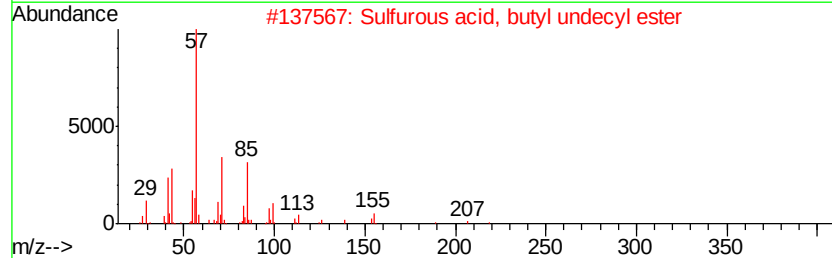
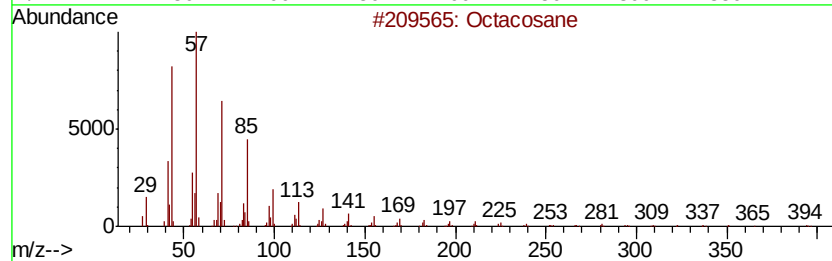
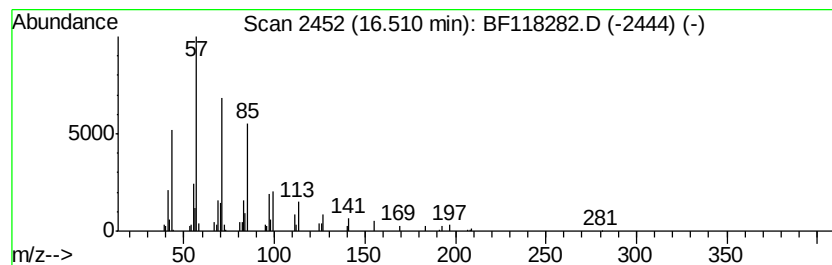
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 Sulfurous acid, butyl undec... Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 16.51 | 2.95 ng | 125186 | Perylene-d12     | 15.54 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | Octacosane                          | 394 | C28H58    | 000630-02-4  | 91   |
| 2    |    | Sulfurous acid, butyl undecyl ester | 292 | C15H32O3S | 1000309-17-8 | 91   |
| 3    |    | 2-methyloctacosane                  | 408 | C29H60    | 1000376-72-8 | 91   |
| 4    |    | 2-methyltetracosane                 | 352 | C25H52    | 1000376-72-6 | 90   |
| 5    |    | Heneicosane                         | 296 | C21H44    | 000629-94-7  | 87   |





Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF121919\  
Data File : BF118282.D  
Acq On : 19 Dec 2019 16:30  
Operator : JU  
Sample : PB125606BL  
Misc :  
ALS Vial : 9 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB125606BL

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF120619.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... | 5.09  | 17.1    | ng    | 577561   | 1                     | 6.86  | 673556 | 20.0 |
| unknown6.63          | 6.63  | 103.8   | ng    | 3494080  | 1                     | 6.86  | 673556 | 20.0 |
| Triacontane          | 14.82 | 3.4     | ng    | 144838   | 6                     | 15.54 | 850037 | 20.0 |
| Octacosane           | 15.16 | 4.0     | ng    | 168314   | 6                     | 15.54 | 850037 | 20.0 |
| Eicosane             | 15.99 | 4.5     | ng    | 191394   | 6                     | 15.54 | 850037 | 20.0 |
| Sulfurous acid, b... | 16.51 | 3.0     | ng    | 125186   | 6                     | 15.54 | 850037 | 20.0 |