

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122322\  
 Data File : BF131814.D  
 Acq On : 23 Dec 2022 19:24  
 Operator : CG\JU  
 Sample : N6157-03  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 20221420-COMPOSITE-C

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-BF122022.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131814.D\data.ms

| 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         | 5.051       | 499           | 504         | 517          | rVB      | 581013         | 703271        | 33.62%          | 4.731%        |
| 2         | 5.457       | 569           | 573         | 576          | rBV      | 1893224        | 1762228       | 84.25%          | 11.854%       |
| 3         | 6.481       | 741           | 747         | 750          | rBV      | 1693644        | 1815874       | 86.82%          | 12.215%       |
| 4         | 6.845       | 805           | 809         | 812          | rBV      | 565342         | 431117        | 20.61%          | 2.900%        |
| 5         | 7.416       | 901           | 906         | 909          | rBV      | 1335026        | 1187793       | 56.79%          | 7.990%        |
| 6         | 8.133       | 1024          | 1028        | 1032         | rBV      | 635414         | 556285        | 26.60%          | 3.742%        |
| 7         | 9.222       | 1208          | 1213        | 1216         | rBV      | 2419893        | 2091630       | 100.00%         | 14.070%       |
| 8         | 9.904       | 1324          | 1329        | 1332         | rBV      | 816996         | 678680        | 32.45%          | 4.565%        |
| 9         | 10.622      | 1448          | 1451        | 1454         | rBV      | 53517          | 40911         | 1.96%           | 0.275%        |
| 10        | 10.698      | 1459          | 1464        | 1467         | rBV      | 1788568        | 1527072       | 73.01%          | 10.272%       |
| 11        | 11.398      | 1579          | 1583        | 1586         | rBV      | 896121         | 722373        | 34.54%          | 4.859%        |
| 12        | 11.927      | 1669          | 1673        | 1678         | rBV      | 113414         | 107000        | 5.12%           | 0.720%        |
| 13        | 12.992      | 1850          | 1854        | 1858         | rBV      | 2102142        | 2016230       | 96.40%          | 13.563%       |
| 14        | 13.892      | 2003          | 2007        | 2011         | rVB      | 23151          | 24359         | 1.16%           | 0.164%        |
| 15        | 13.980      | 2014          | 2022        | 2031         | rBV7     | 39811          | 160369        | 7.67%           | 1.079%        |
| 16        | 14.057      | 2031          | 2035        | 2038         | rVB      | 577752         | 506023        | 24.19%          | 3.404%        |
| 17        | 14.151      | 2047          | 2051        | 2057         | rVB      | 33391          | 38385         | 1.84%           | 0.258%        |
| 18        | 14.215      | 2057          | 2062        | 2070         | rBV2     | 20995          | 23051         | 1.10%           | 0.155%        |
| 19        | 14.521      | 2109          | 2114        | 2120         | rBV      | 25441          | 25884         | 1.24%           | 0.174%        |
| 20        | 14.909      | 2177          | 2180        | 2187         | rVB      | 25929          | 28423         | 1.36%           | 0.191%        |
| 21        | 15.551      | 2284          | 2289        | 2297         | rBV2     | 315946         | 419096        | 20.04%          | 2.819%        |

Sum of corrected areas: 14866054



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122322\  
Data File : BF131814.D  
Acq On : 23 Dec 2022 19:24  
Operator : CG\JU  
Sample : N6157-03  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20221420-COMPOSITE-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

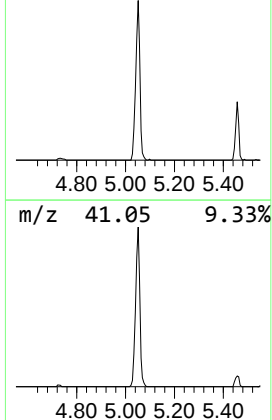
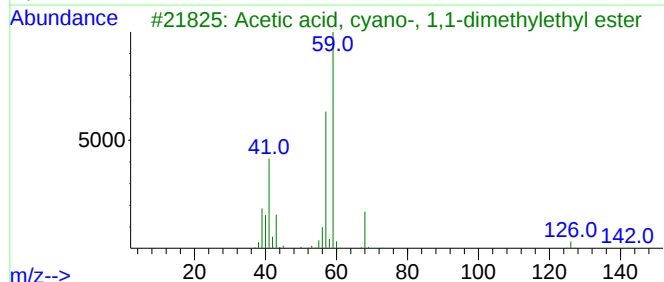
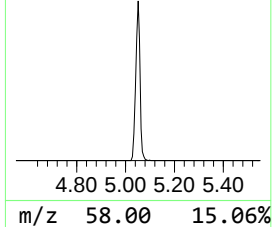
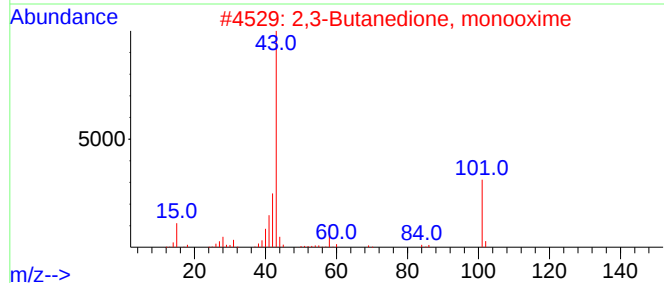
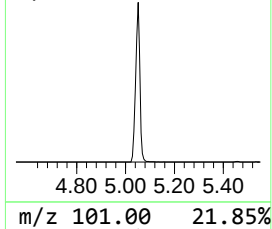
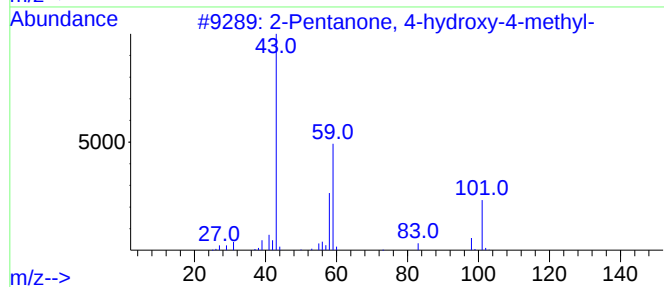
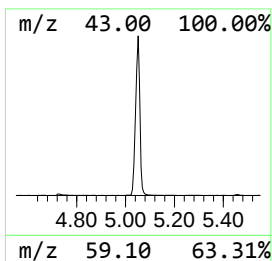
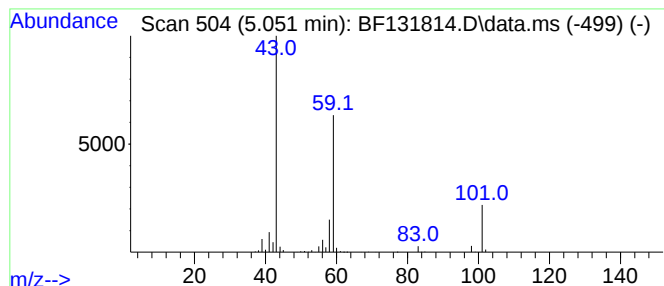
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.051 | 32.63 ng | 703271 | 1,4-Dichlorobenzene-d4 | 6.845 |

| 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-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 23      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Butane, 1-ethoxy-                   | 102 | C6H14O       | 000628-81-9 | 9       |      |      |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122322\  
Data File : BF131814.D  
Acq On : 23 Dec 2022 19:24  
Operator : CG\JU  
Sample : N6157-03  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20221420-COMPOSITE-C

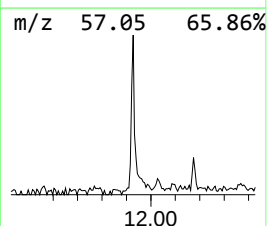
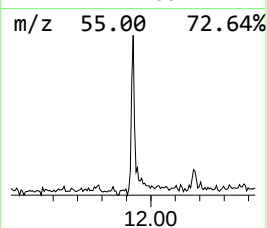
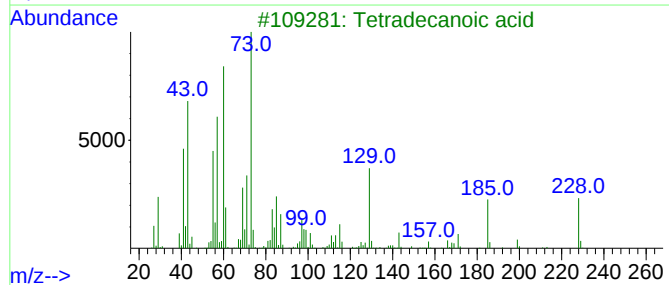
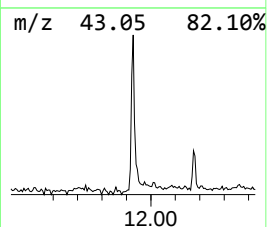
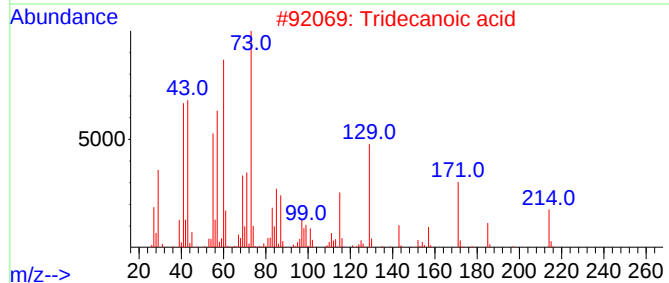
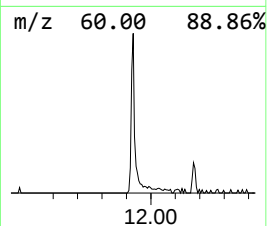
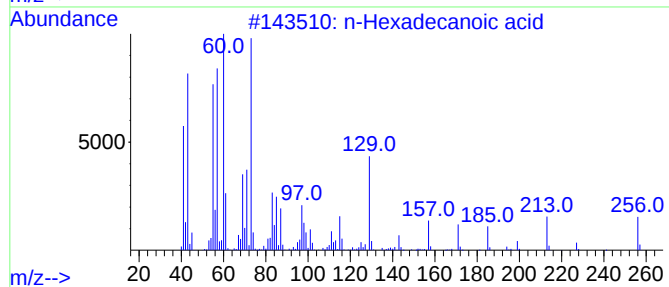
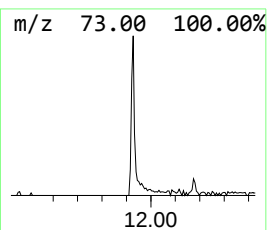
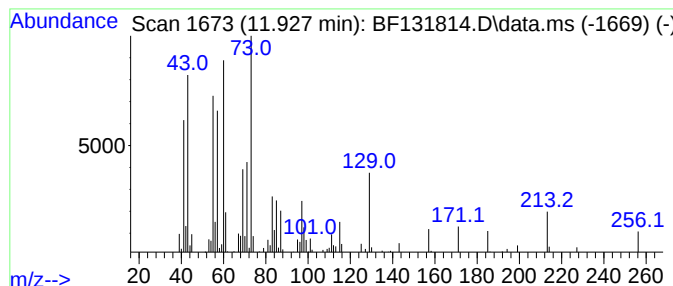
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.927 | 2.96 ng | 107000 | Phenanthrene-d10 | 11.398 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 95   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 80   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 76   |
| 5    |    |   | Nonanoic acid       | 158 | C9H18O2  | 000112-05-0 | 45   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122322\  
Data File : BF131814.D  
Acq On : 23 Dec 2022 19:24  
Operator : CG\JU  
Sample : N6157-03  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20221420-COMPOSITE-C

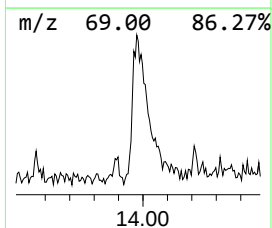
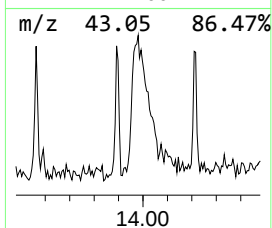
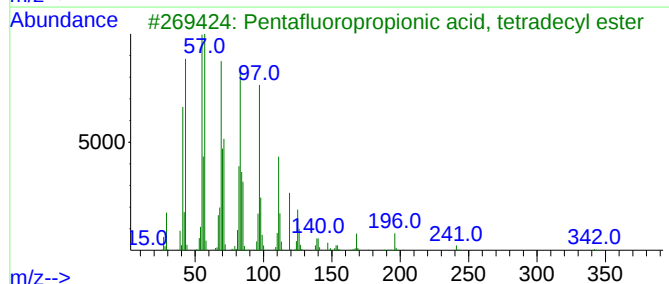
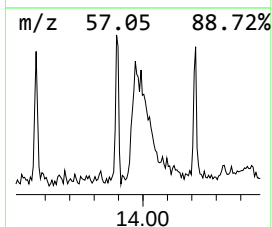
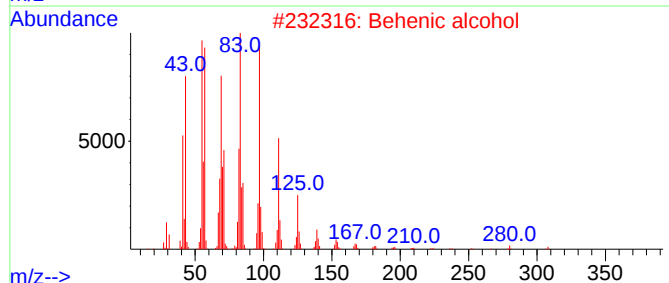
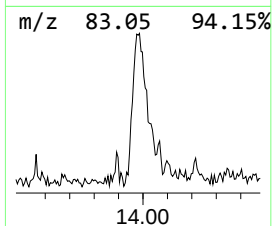
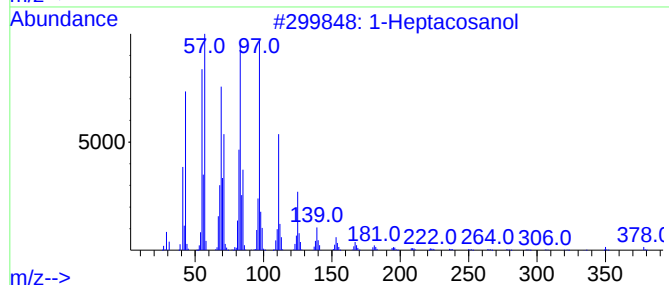
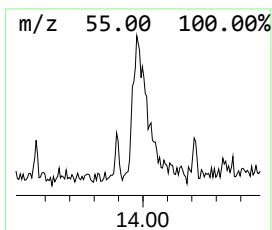
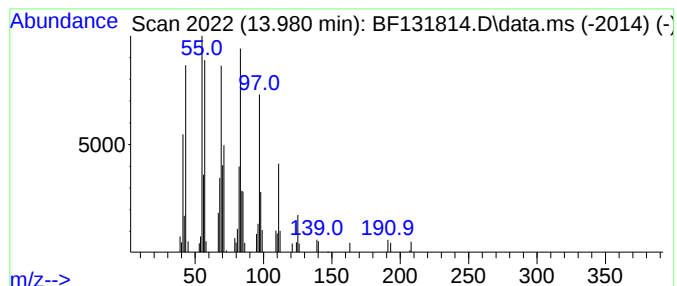
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*

Peak Number 3 1-Heptacosanol Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 13.980    | 6.34 ng                             | 160369 | Chrysene-d12     | 14.057      |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Heptacosanol                      | 396    | C27H56O          | 002004-39-9 | 94   |
| 2         | Behenic alcohol                     | 326    | C22H46O          | 000661-19-8 | 91   |
| 3         | Pentafluoropropionic acid, tetra... | 360    | C17H29F5O2       | 006222-06-6 | 91   |
| 4         | n-Tetracosanol-1                    | 354    | C24H50O          | 000506-51-4 | 91   |
| 5         | Heptafluorobutyric acid, n-tetra... | 410    | C18H29F7O2       | 007365-36-8 | 91   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF122322\  
Data File : BF131814.D  
Acq On : 23 Dec 2022 19:24  
Operator : CG\JU  
Sample : N6157-03  
Misc :  
ALS Vial : 15 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
20221420-COMPOSITE-C

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF122022.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.051  | 32.6    | ng    | 703271   | 1                     | 6.845  | 431117 | 20.0 |
| n-Hexadecanoic ... | 11.927 | 3.0     | ng    | 107000   | 4                     | 11.398 | 722373 | 20.0 |
| 1-Heptacosanol     | 13.980 | 6.3     | ng    | 160369   | 5                     | 14.057 | 506023 | 20.0 |