

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042423\  
 Data File : BF132996.D  
 Acq On : 24 Apr 2023 15:38  
 Operator : CG\JU  
 Sample : 02469-03  
 Misc :  
 ALS Vial : 10 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TWP-24

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-BF042123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132996.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         | 4.928       | 475           | 483         | 487          | rBV      | 1256756        | 1360678       | 24.51%          | 3.946%        |
| 2         | 5.351       | 551           | 555         | 558          | rBV      | 1977601        | 1660404       | 29.91%          | 4.815%        |
| 3         | 6.340       | 716           | 723         | 725          | rBV      | 46195          | 62361         | 1.12%           | 0.181%        |
| 4         | 6.375       | 725           | 729         | 732          | rBV      | 1382638        | 1060925       | 19.11%          | 3.077%        |
| 5         | 6.745       | 788           | 792         | 795          | rBV      | 1725197        | 1359702       | 24.50%          | 3.943%        |
| 6         | 7.310       | 882           | 888         | 891          | rBV      | 3744106        | 3463095       | 62.39%          | 10.043%       |
| 7         | 8.028       | 1006          | 1010        | 1013         | rBV      | 2429055        | 1890746       | 34.06%          | 5.483%        |
| 8         | 9.110       | 1188          | 1194        | 1197         | rBV      | 6191649        | 5550767       | 100.00%         | 16.098%       |
| 9         | 9.369       | 1235          | 1238        | 1242         | rBV      | 166556         | 115445        | 2.08%           | 0.335%        |
| 10        | 9.781       | 1304          | 1308        | 1311         | rBV      | 2736672        | 2096726       | 37.77%          | 6.081%        |
| 11        | 10.098      | 1359          | 1362        | 1369         | rVB      | 197382         | 173466        | 3.13%           | 0.503%        |
| 12        | 10.492      | 1425          | 1429        | 1432         | rBV      | 850695         | 640011        | 11.53%          | 1.856%        |
| 13        | 10.569      | 1437          | 1442        | 1445         | rBV      | 2707328        | 2360950       | 42.53%          | 6.847%        |
| 14        | 11.263      | 1556          | 1560        | 1563         | rBV      | 2428989        | 2052421       | 36.98%          | 5.952%        |
| 15        | 11.804      | 1648          | 1652        | 1662         | rBV      | 1017299        | 1001694       | 18.05%          | 2.905%        |
| 16        | 12.586      | 1781          | 1785        | 1794         | rBV      | 356434         | 370251        | 6.67%           | 1.074%        |
| 17        | 12.851      | 1826          | 1830        | 1834         | rBV      | 5241557        | 5349497       | 96.37%          | 15.514%       |
| 18        | 13.774      | 1983          | 1987        | 1999         | rVB      | 332370         | 585709        | 10.55%          | 1.699%        |
| 19        | 13.898      | 2004          | 2008        | 2011         | rBV      | 1791391        | 1519064       | 27.37%          | 4.405%        |
| 20        | 13.998      | 2019          | 2025        | 2037         | rVB      | 145194         | 185084        | 3.33%           | 0.537%        |
| 21        | 14.757      | 2151          | 2154        | 2158         | rVB      | 213526         | 196462        | 3.54%           | 0.570%        |
| 22        | 15.321      | 2245          | 2250        | 2256         | rVB      | 1101313        | 1268626       | 22.85%          | 3.679%        |
| 23        | 15.886      | 2340          | 2346        | 2359         | rVB6     | 46239          | 157211        | 2.83%           | 0.456%        |

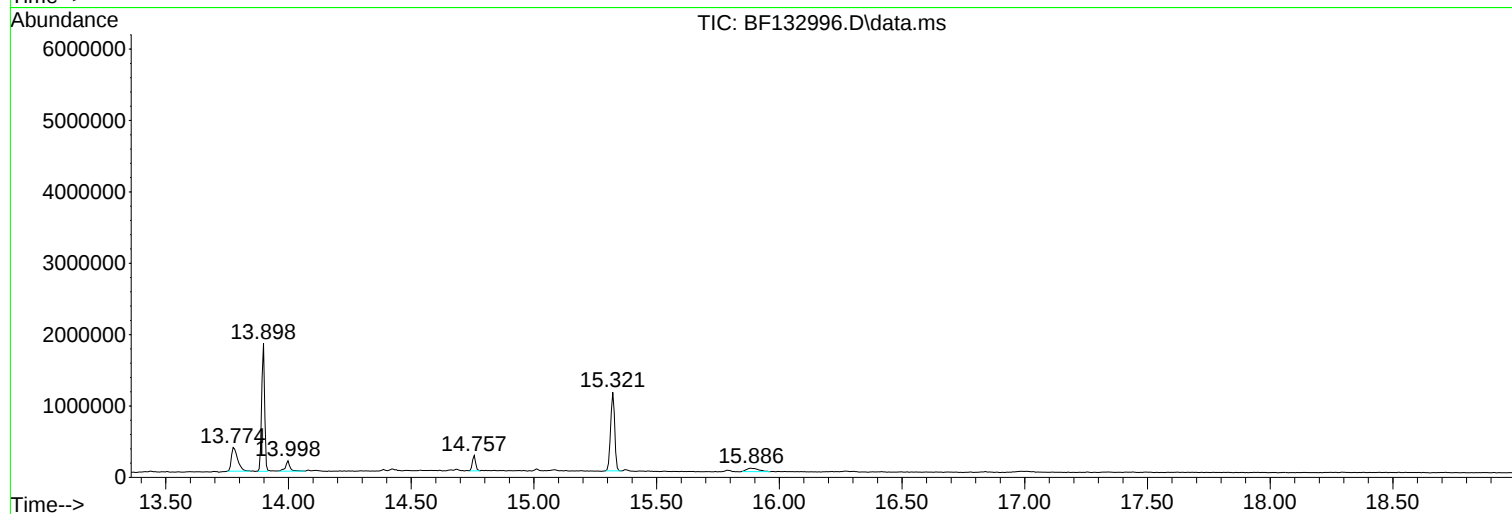
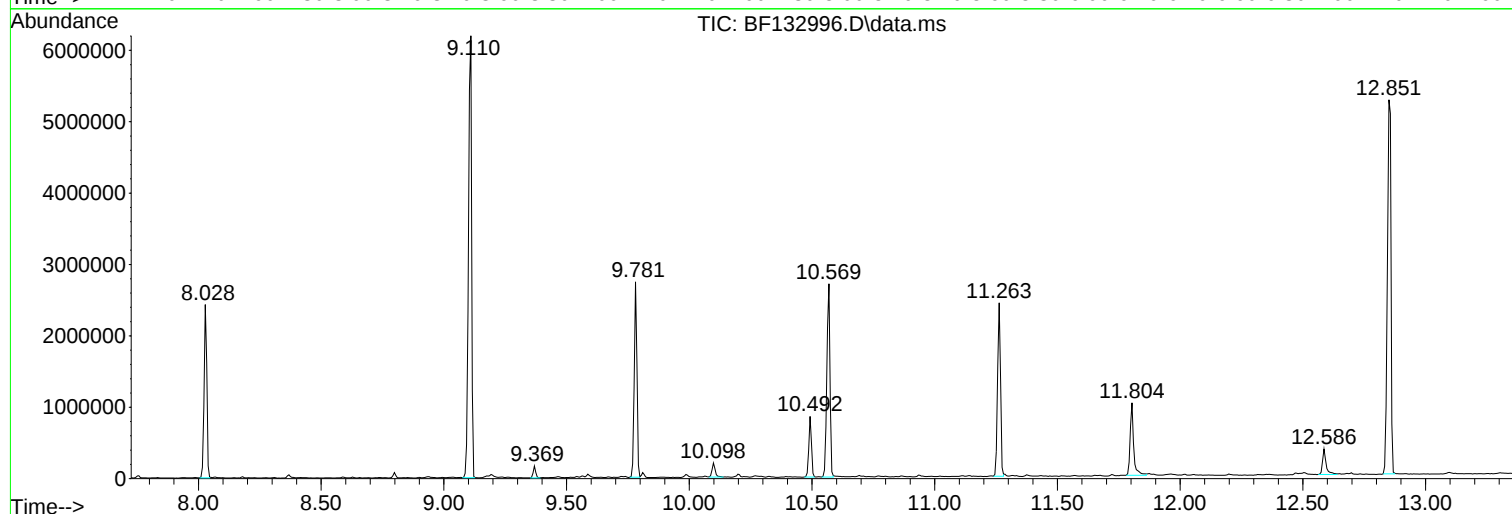
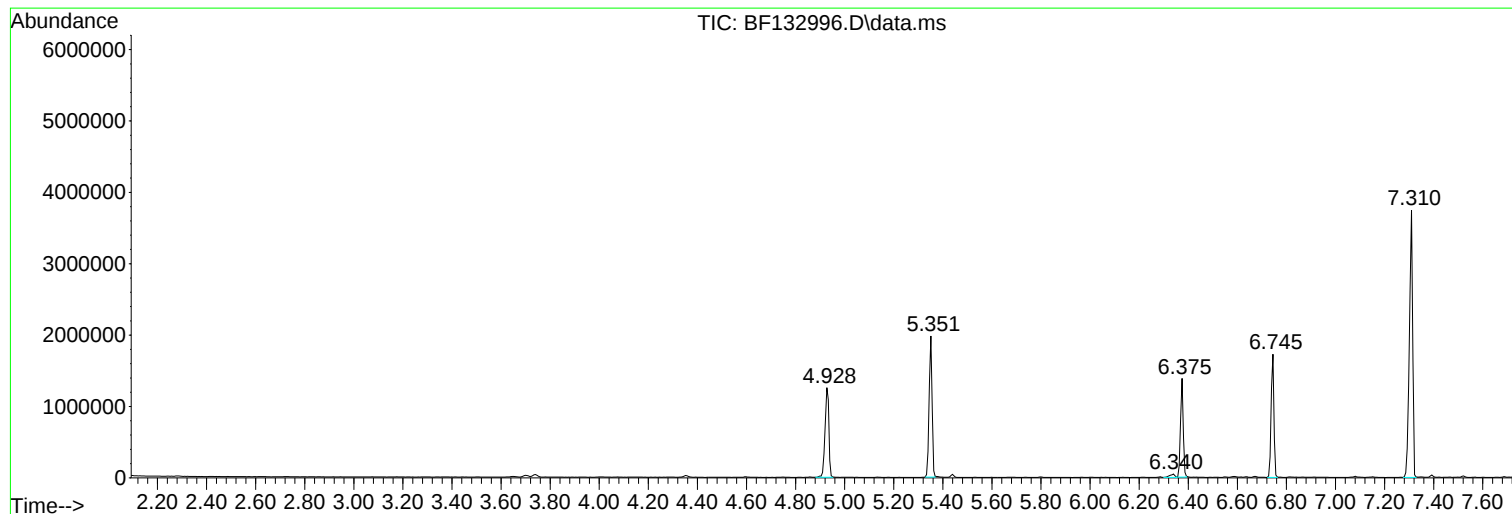
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BNA\_F  
ClientSampleId :  
TWP-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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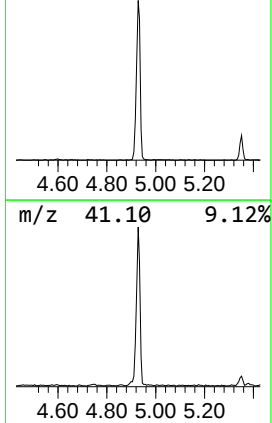
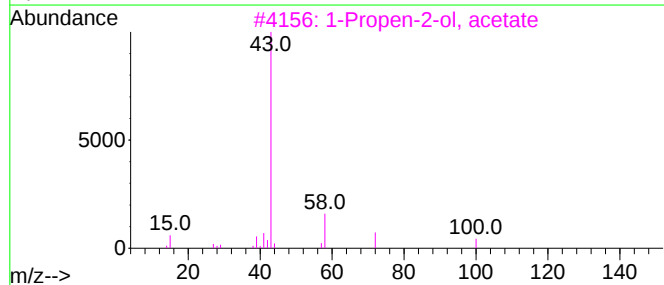
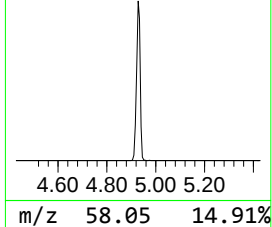
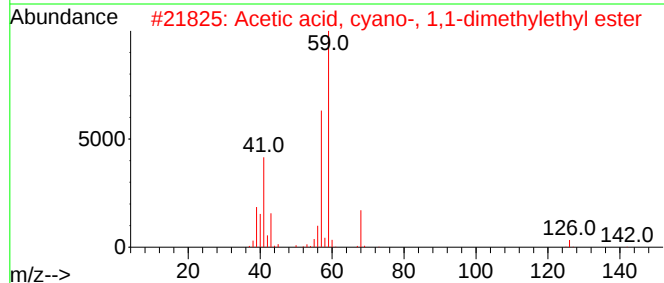
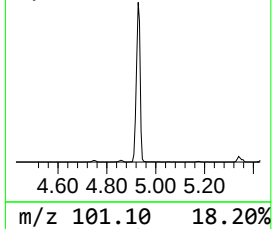
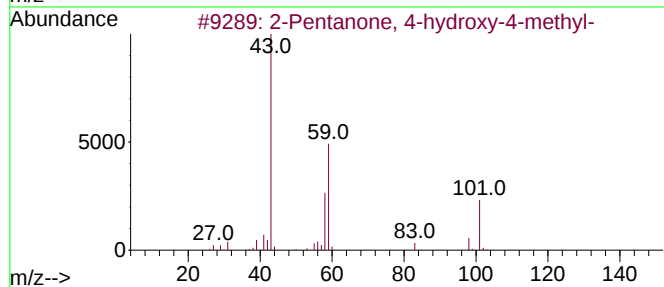
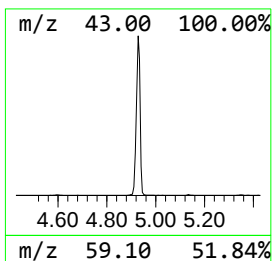
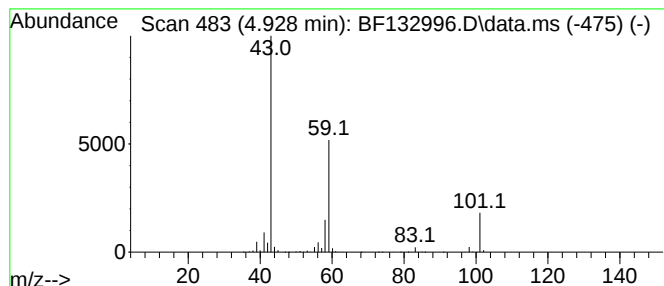
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.      | EstConc                             | Area    | Relative to ISTD       | R.T.        |      |
|-----------|-------------------------------------|---------|------------------------|-------------|------|
| 4.928     | 20.01 ng                            | 1360680 | 1,4-Dichlorobenzene-d4 | 6.745       |      |
| Hit# of 5 | Tentative ID                        | MW      | MolForm                | CAS#        | Qual |
| 1         | 2-Pentanone, 4-hydroxy-4-methyl-    | 116     | C6H12O2                | 000123-42-2 | 56   |
| 2         | Acetic acid, cyano-, 1,1-dimethy... | 141     | C7H11NO2               | 001116-98-9 | 25   |
| 3         | 1-Propen-2-ol, acetate              | 100     | C5H8O2                 | 000108-22-5 | 12   |
| 4         | 2,3-Butanedione, monooxime          | 101     | C4H7NO2                | 000057-71-6 | 9    |
| 5         | 3-Hexanol, 4-ethyl-                 | 130     | C8H18O                 | 019780-44-0 | 9    |



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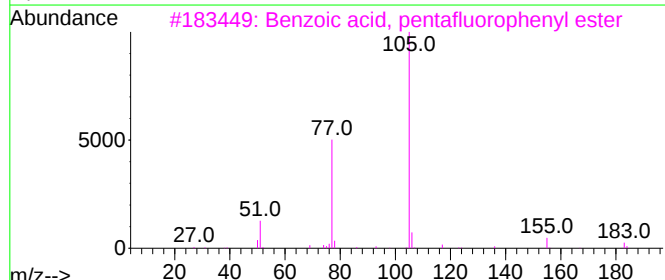
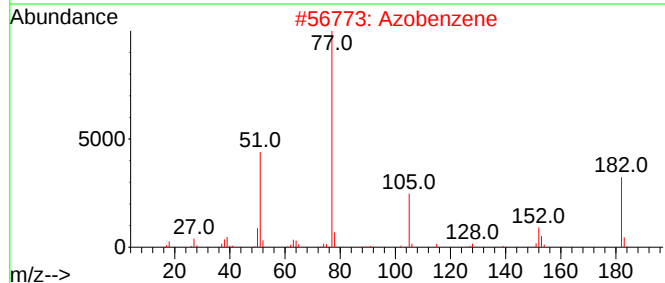
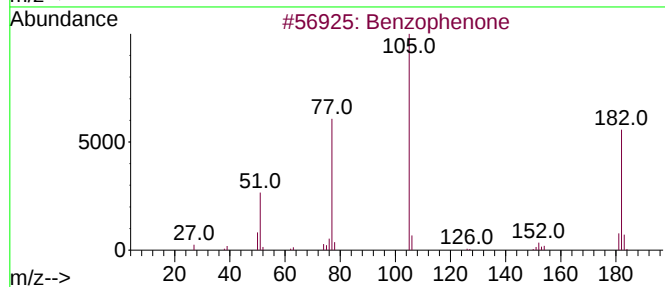
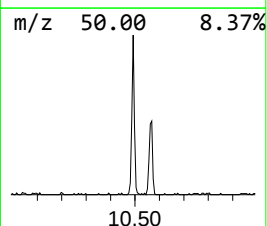
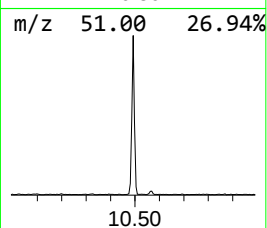
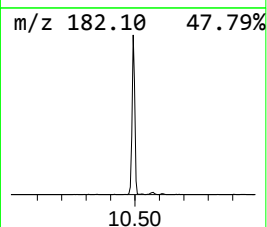
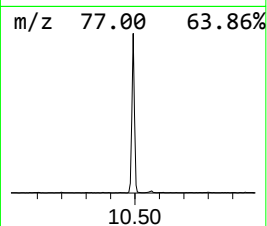
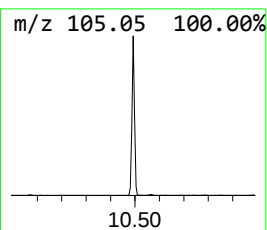
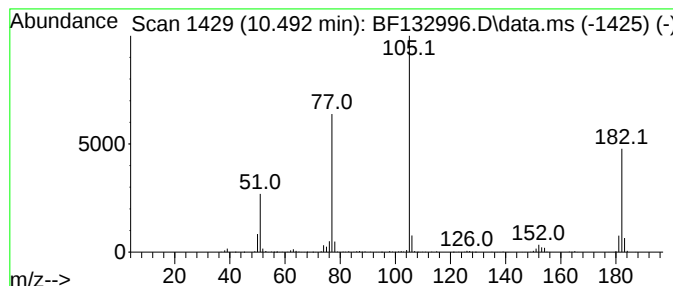
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzophenone Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.492 | 6.10 ng | 640011 | Acenaphthene-d10 | 9.781 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Benzophenone                        | 182 | C13H10O    | 000119-61-9  | 96   |
| 2    |    |   | Azobenzene                          | 182 | C12H10N2   | 000103-33-3  | 64   |
| 3    |    |   | Benzoic acid, pentafluorophenyl ... | 288 | C13H5F5O2  | 1000360-67-9 | 50   |
| 4    |    |   | N-Methylbenzamide, N-trifluoroac... | 231 | C10H8F3NO2 | 1000446-91-5 | 47   |
| 5    |    |   | 1-Propanone, 3-chloro-1-phenyl-     | 168 | C9H9ClO    | 000936-59-4  | 47   |



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TWP-24

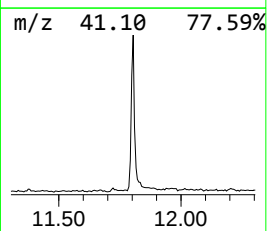
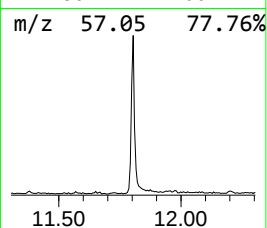
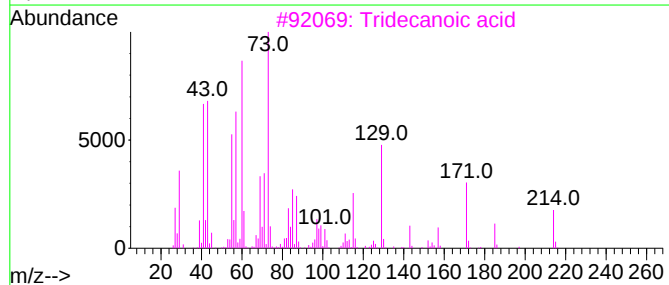
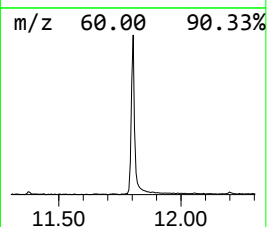
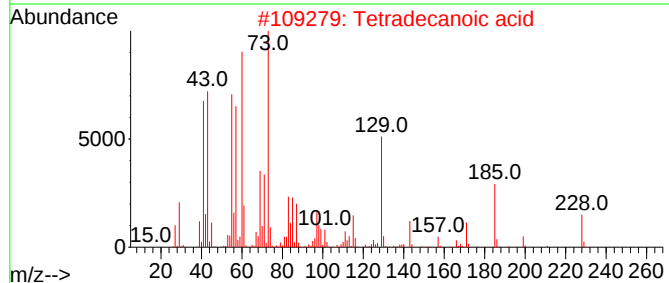
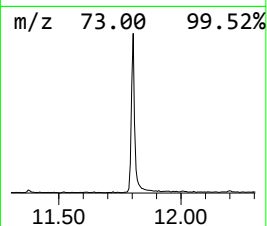
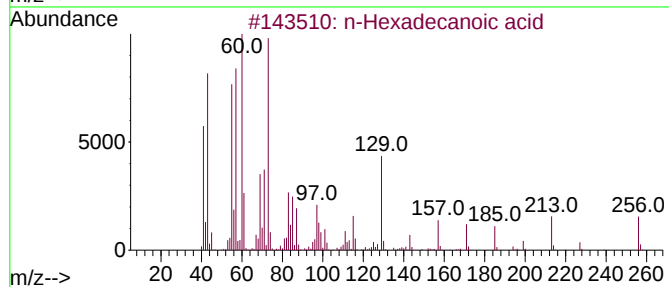
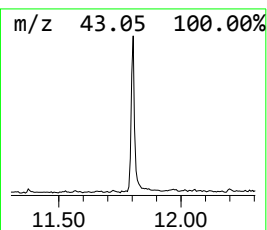
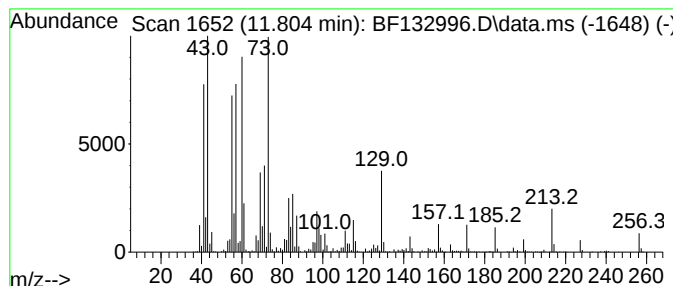
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area    | Relative to ISTD | R.T.   |
|--------|---------|---------|------------------|--------|
| 11.804 | 9.76 ng | 1001690 | Phenanthrene-d10 | 11.263 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 97   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 96   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 64   |



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BNA\_F  
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TWP-24

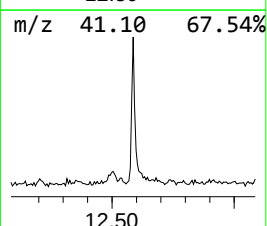
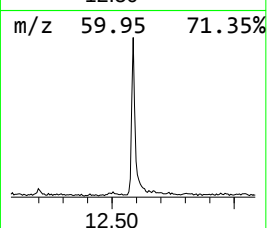
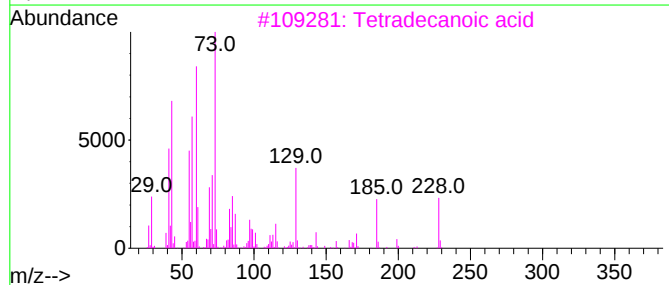
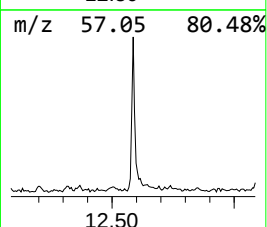
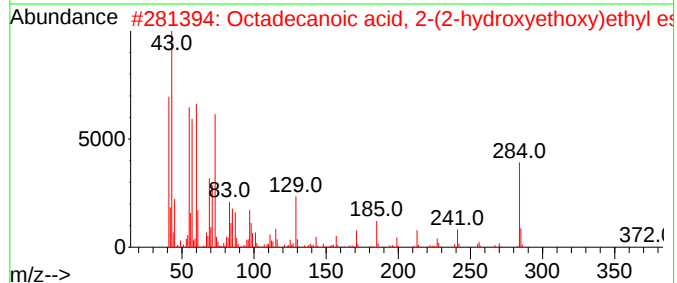
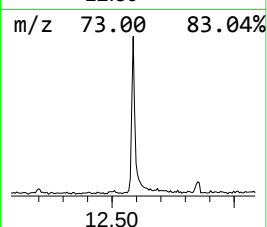
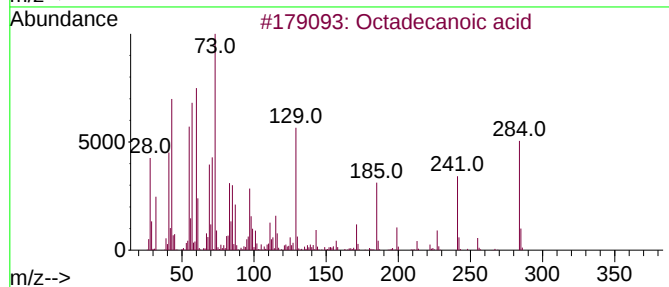
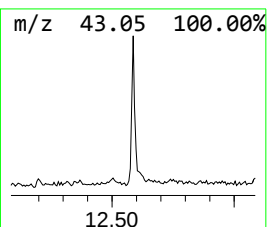
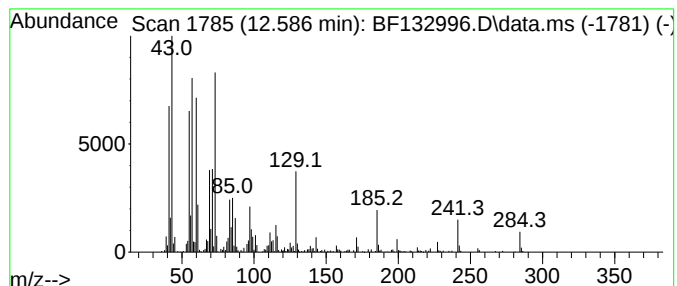
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.586 | 4.87 ng | 370251 | Chrysene-d12     | 13.898 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 87   |
| 3    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 4    |    |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5 | 86   |
| 5    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 83   |



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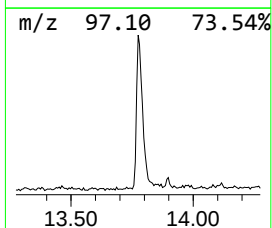
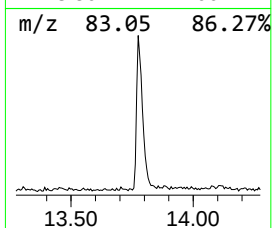
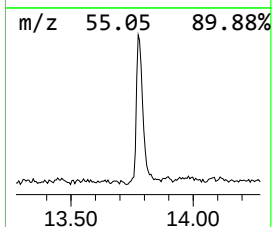
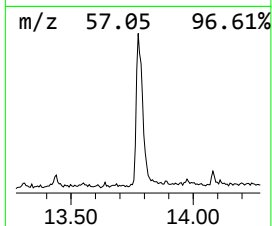
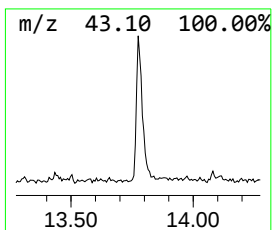
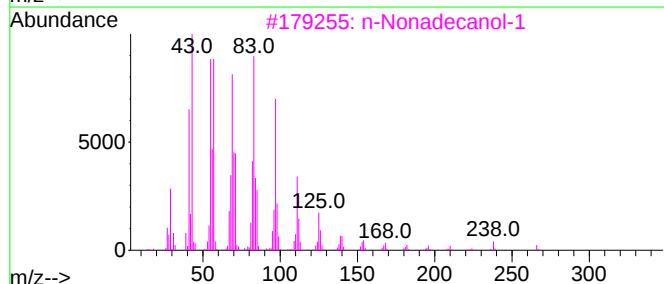
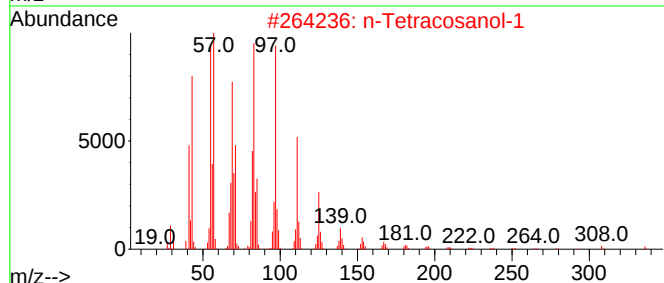
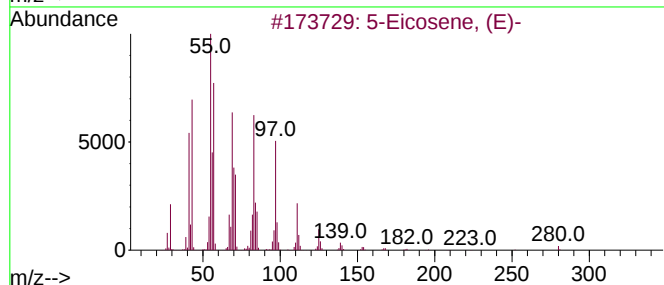
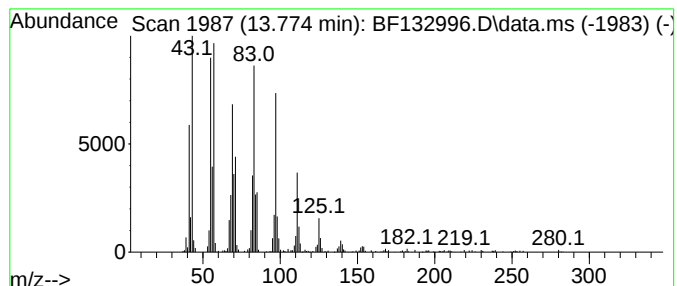
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 5-Eicosene, (E)- Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.774 | 7.71 ng | 585709 | Chrysene-d12     | 13.898 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|------------|-------------|------|
| 1    |    |   | 5-Eicosene, (E)-                  | 280 | C20H40     | 074685-30-6 | 99   |
| 2    |    |   | n-Tetracosanol-1                  | 354 | C24H50O    | 000506-51-4 | 94   |
| 3    |    |   | n-Nonadecanol-1                   | 284 | C19H40O    | 001454-84-8 | 94   |
| 4    |    |   | Bromoacetic acid, hexadecyl ester | 362 | C18H35BrO2 | 005454-48-8 | 94   |
| 5    |    |   | 1-Heneicosanol                    | 312 | C21H44O    | 015594-90-8 | 93   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042423\  
Data File : BF132996.D  
Acq On : 24 Apr 2023 15:38  
Operator : CG\JU  
Sample : 02469-03  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TWP-24

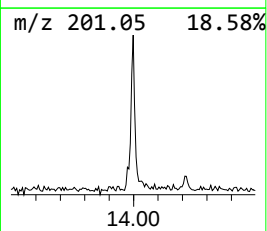
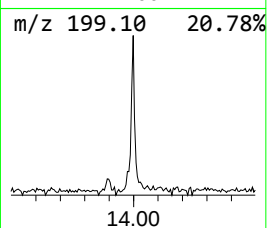
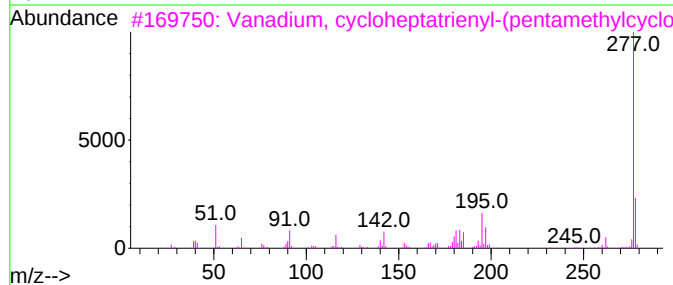
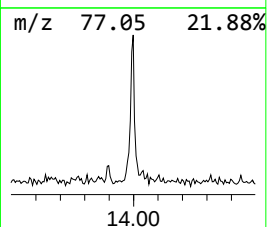
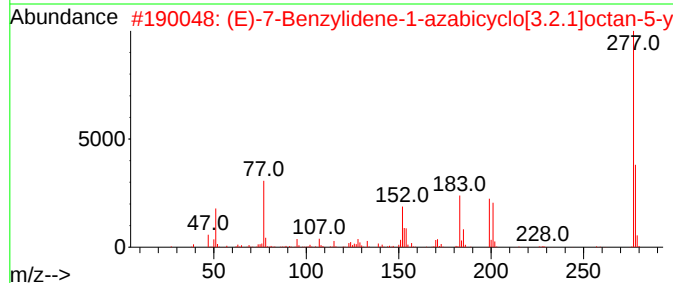
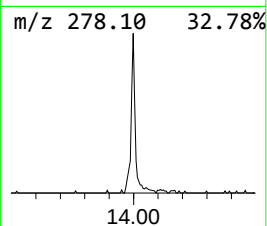
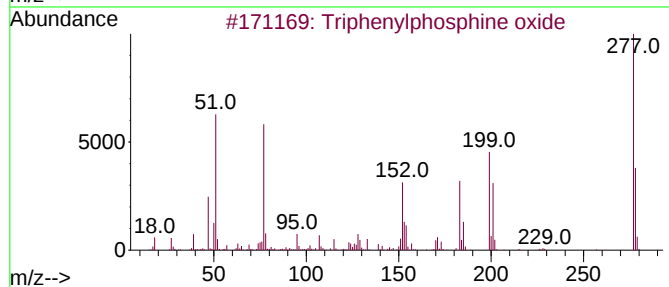
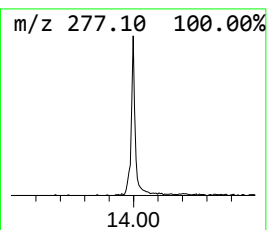
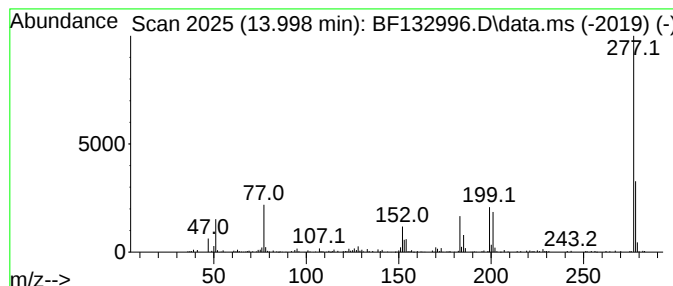
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 6 Triphenylphosphine oxide Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.998 | 2.44 ng | 185084 | Chrysene-d12     | 13.898 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide            | 278 | C18H15OP   | 000791-28-6  | 95   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3... | 293 | C15H19NO3S | 1000483-83-4 | 64   |
| 3    |    |   | Vanadium, cycloheptatrienyl-(pen... | 277 | C17H22V    | 1000155-20-5 | 47   |
| 4    |    |   | Formaldehyde, (triphenylphosphor... | 304 | C19H17N2P  | 015990-54-2  | 45   |
| 5    |    |   | 5-quinolinol, 8-[2-(3,5-dimethyl... | 277 | C17H15N3O  | 1000397-10-2 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042423\  
Data File : BF132996.D  
Acq On : 24 Apr 2023 15:38  
Operator : CG\JU  
Sample : 02469-03  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TWP-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

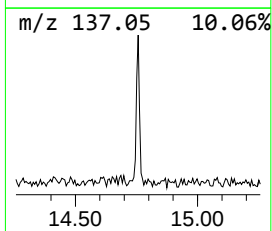
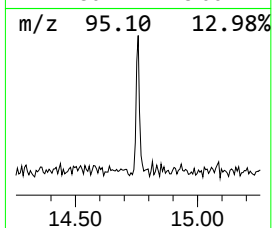
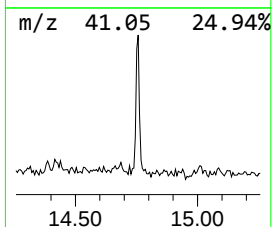
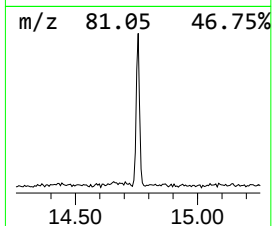
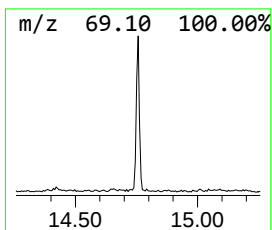
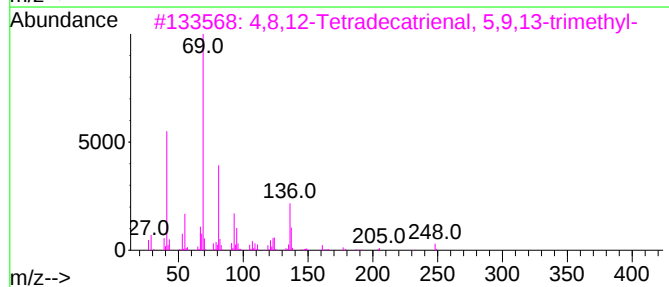
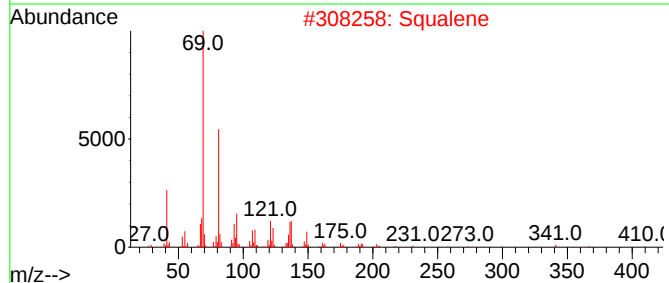
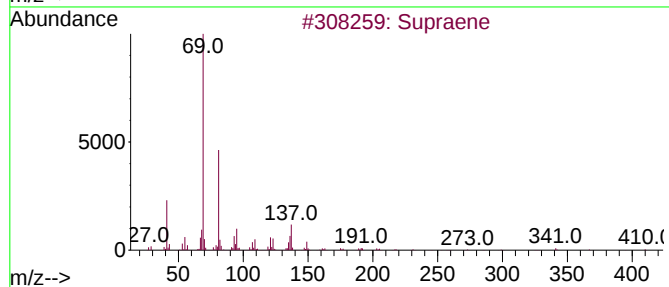
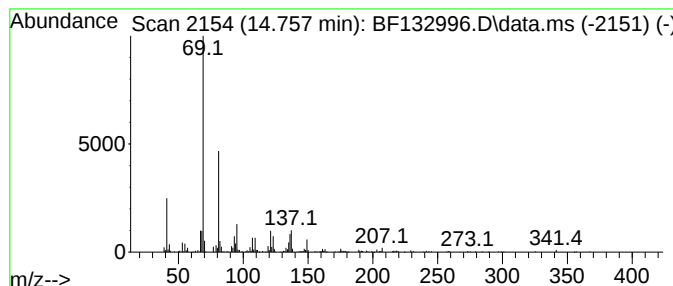
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Supraene Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.757 | 3.10 ng | 196462 | Perylene-d12     | 15.321 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50   | 007683-64-9 | 91   |
| 2    |    |   | Squalene                            | 410 | C30H50   | 000111-02-4 | 91   |
| 3    |    |   | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O  | 066408-55-7 | 72   |
| 4    |    |   | Furan, 3-(4,8-dimethyl-3,7-nonad... | 218 | C15H22O  | 023262-34-2 | 59   |
| 5    |    |   | 1,3-Dioxolan-2-one, 3-methyl-3-(... | 264 | C16H24O3 | 336879-76-6 | 53   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042423\  
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Acq On : 24 Apr 2023 15:38  
Operator : CG\JU  
Sample : 02469-03  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TWP-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

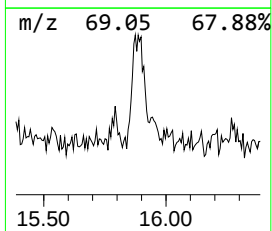
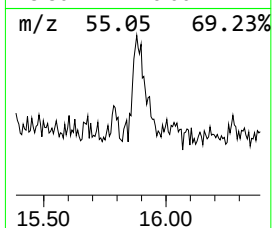
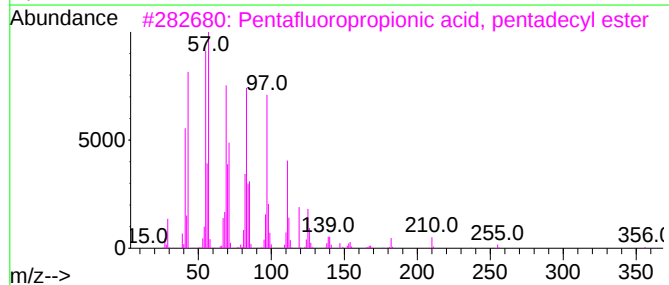
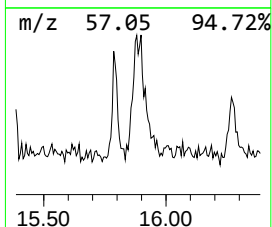
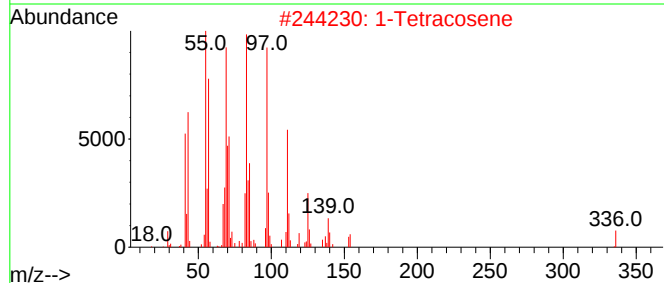
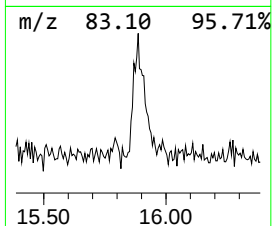
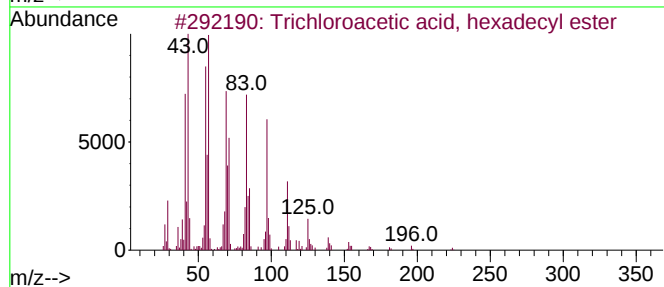
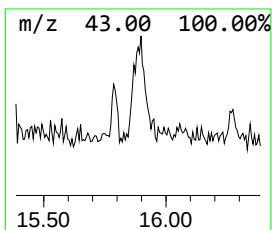
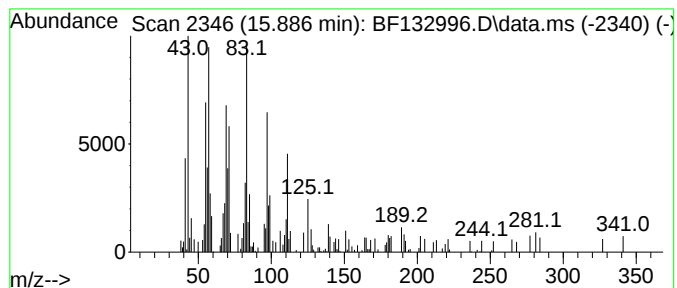
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Trichloroacetic acid, hexad... Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.886 | 2.48 ng | 157211 | Perylene-d12     | 15.321 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-------------|-------------|------|
| 1    |    |   | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 86   |
| 2    |    |   | 1-Tetracosene                       | 336 | C24H48      | 010192-32-2 | 83   |
| 3    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2  | 959092-08-1 | 83   |
| 4    |    |   | Triacontan-15-ol                    | 438 | C30H62O     | 031849-26-0 | 81   |
| 5    |    |   | 1-Hexadecanesulfonyl chloride       | 324 | C16H33ClO2S | 038775-38-1 | 80   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042423\  
Data File : BF132996.D  
Acq On : 24 Apr 2023 15:38  
Operator : CG\JU  
Sample : 02469-03  
Misc :  
ALS Vial : 10 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
TWP-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF042123.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-... | 4.928  | 20.0    | ng    | 1360680  | 1                     | 6.745  | 1359700 | 20.0 |
| Benzophenone       | 10.492 | 6.1     | ng    | 640011   | 3                     | 9.781  | 2096730 | 20.0 |
| n-Hexadecanoic ... | 11.804 | 9.8     | ng    | 1001690  | 4                     | 11.263 | 2052420 | 20.0 |
| Octadecanoic acid  | 12.586 | 4.9     | ng    | 370251   | 5                     | 13.898 | 1519060 | 20.0 |
| 5-Eicosene, (E)-   | 13.774 | 7.7     | ng    | 585709   | 5                     | 13.898 | 1519060 | 20.0 |
| Triphenylphosph... | 13.998 | 2.4     | ng    | 185084   | 5                     | 13.898 | 1519060 | 20.0 |
| Supraene           | 14.757 | 3.1     | ng    | 196462   | 6                     | 15.321 | 1268630 | 20.0 |
| Trichloroacetic... | 15.886 | 2.5     | ng    | 157211   | 6                     | 15.321 | 1268630 | 20.0 |