

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052722\  
 Data File : BF128519.D  
 Acq On : 27 May 2022 19:57  
 Operator : CG\JU  
 Sample : N2922-25  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 P024-SS004-0006-01

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-BF052622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128519.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         | 4.416       | 358           | 362         | 373          | rBV2     | 55795          | 72069         | 1.20%           | 0.167%        |
| 2         | 4.857       | 431           | 437         | 445          | rBV      | 57566          | 67198         | 1.12%           | 0.156%        |
| 3         | 5.081       | 471           | 475         | 481          | rVB      | 75191          | 97559         | 1.63%           | 0.227%        |
| 4         | 5.457       | 533           | 539         | 542          | rBV      | 4605959        | 5066150       | 84.69%          | 11.768%       |
| 5         | 6.463       | 703           | 710         | 713          | rBV      | 4286788        | 5133344       | 85.82%          | 11.924%       |
| 6         | 6.575       | 726           | 729         | 732          | rVB      | 91788          | 69720         | 1.17%           | 0.162%        |
| 7         | 6.834       | 770           | 773         | 777          | rVB      | 1580413        | 1393447       | 23.29%          | 3.237%        |
| 8         | 7.398       | 863           | 869         | 872          | rBV      | 3462598        | 3468365       | 57.98%          | 8.057%        |
| 9         | 8.116       | 986           | 991         | 995          | rBV      | 1887140        | 1834398       | 30.67%          | 4.261%        |
| 10        | 9.198       | 1168          | 1175        | 1178         | rBV      | 5802805        | 5981786       | 100.00%         | 13.895%       |
| 11        | 9.875       | 1284          | 1290        | 1293         | rBV      | 2342178        | 2081499       | 34.80%          | 4.835%        |
| 12        | 10.663      | 1417          | 1424        | 1427         | rBV      | 3800250        | 3631209       | 60.70%          | 8.435%        |
| 13        | 11.363      | 1538          | 1543        | 1546         | rBV      | 2305634        | 2046370       | 34.21%          | 4.754%        |
| 14        | 11.857      | 1623          | 1627        | 1629         | rBV      | 95886          | 103637        | 1.73%           | 0.241%        |
| 15        | 11.892      | 1629          | 1633        | 1645         | rVB      | 653587         | 663110        | 11.09%          | 1.540%        |
| 16        | 12.680      | 1763          | 1767        | 1780         | rVB      | 228756         | 261192        | 4.37%           | 0.607%        |
| 17        | 12.957      | 1809          | 1814        | 1817         | rVB      | 5121249        | 5357058       | 89.56%          | 12.444%       |
| 18        | 13.892      | 1965          | 1973        | 1986         | rBV3     | 142624         | 494719        | 8.27%           | 1.149%        |
| 19        | 13.998      | 1987          | 1991        | 1995         | rBV      | 1676489        | 1593778       | 26.64%          | 3.702%        |
| 20        | 14.098      | 2001          | 2008        | 2014         | rBV      | 1001144        | 1211711       | 20.26%          | 2.815%        |
| 21        | 15.133      | 2180          | 2184        | 2187         | rBV      | 69589          | 77788         | 1.30%           | 0.181%        |
| 22        | 15.463      | 2235          | 2240        | 2246         | rBV2     | 1017035        | 1240750       | 20.74%          | 2.882%        |
| 23        | 15.957      | 2319          | 2324        | 2332         | rVB      | 90843          | 146176        | 2.44%           | 0.340%        |
| 24        | 16.080      | 2337          | 2345        | 2362         | rBV      | 37142          | 177691        | 2.97%           | 0.413%        |
| 25        | 16.757      | 2456          | 2460        | 2467         | rVB4     | 37901          | 64821         | 1.08%           | 0.151%        |
| 26        | 17.062      | 2507          | 2512        | 2519         | rVB2     | 51912          | 117440        | 1.96%           | 0.273%        |
| 27        | 17.180      | 2524          | 2532        | 2536         | rBV9     | 39774          | 120183        | 2.01%           | 0.279%        |
| 28        | 17.286      | 2545          | 2550        | 2558         | rVB3     | 161886         | 339847        | 5.68%           | 0.789%        |
| 29        | 17.586      | 2595          | 2601        | 2609         | rBV3     | 36769          | 135804        | 2.27%           | 0.315%        |

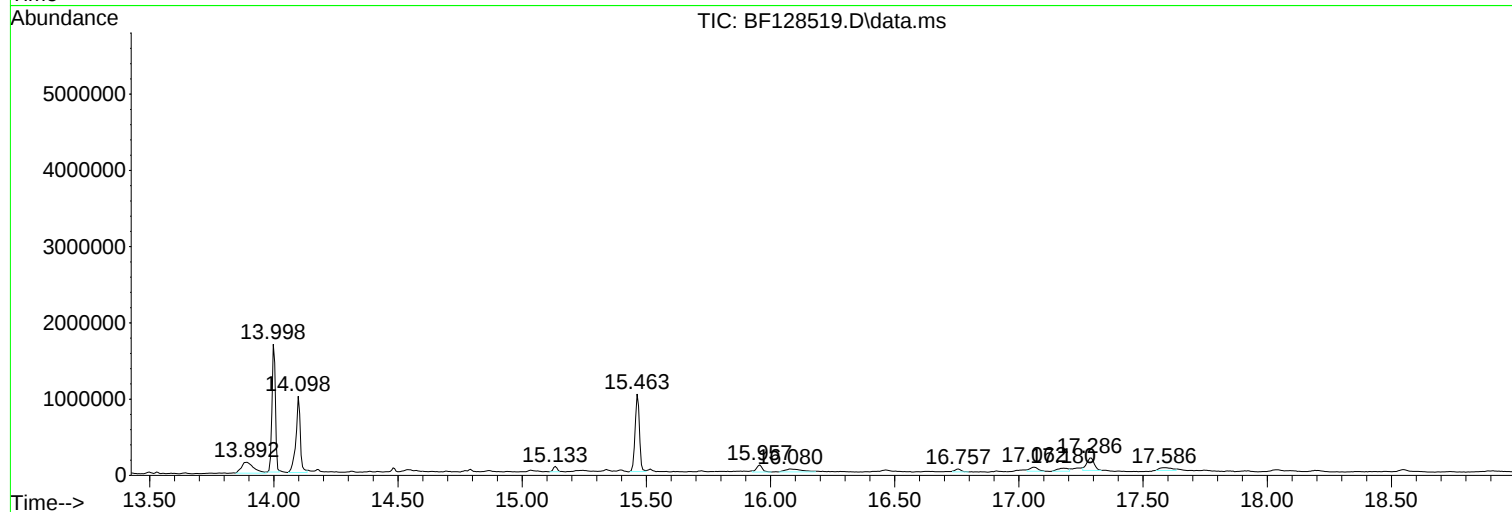
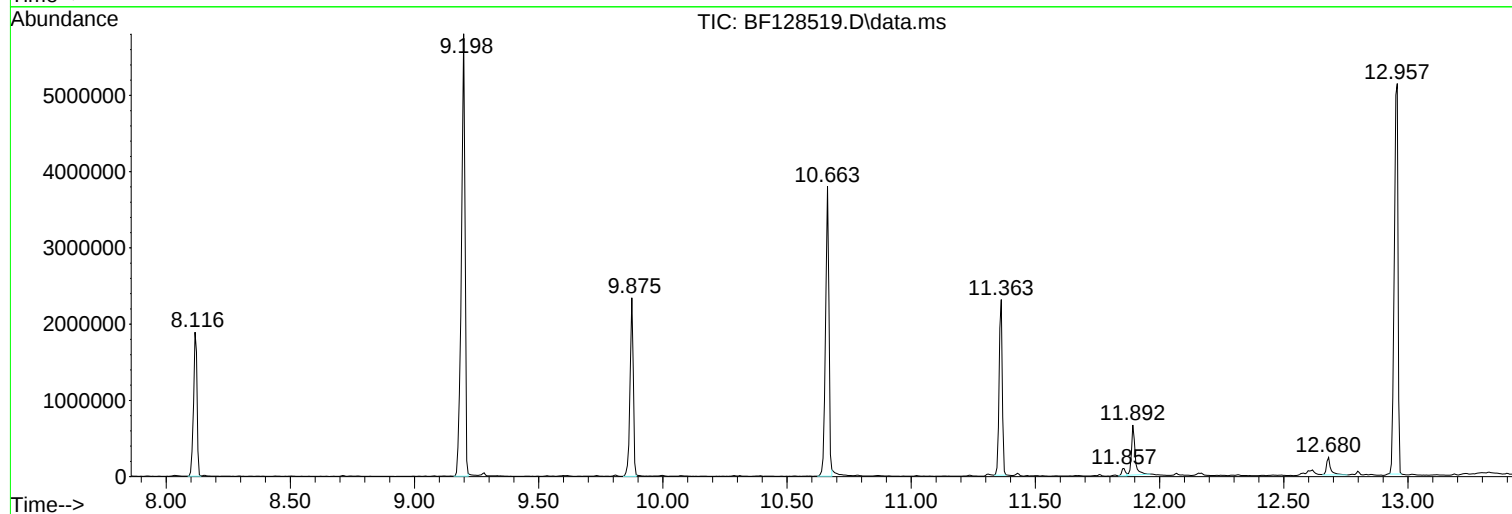
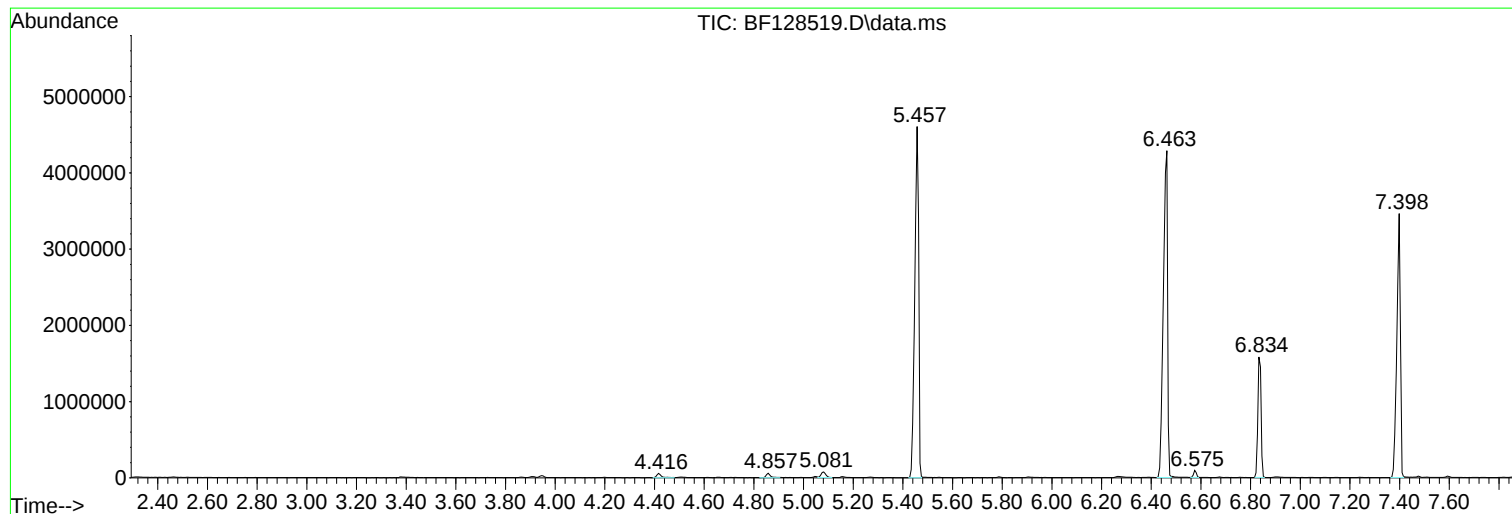
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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.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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Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

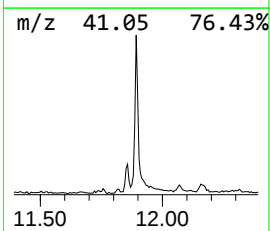
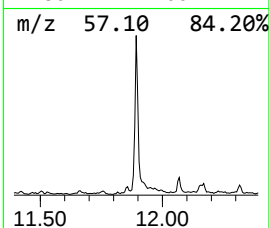
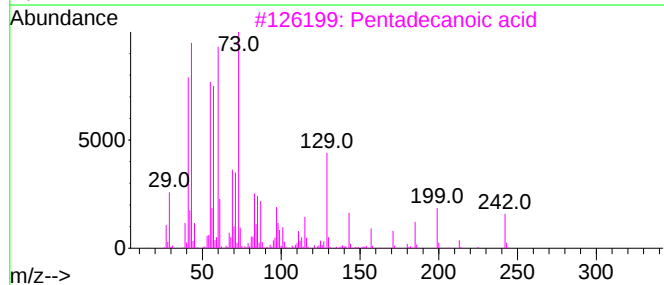
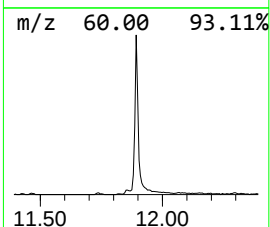
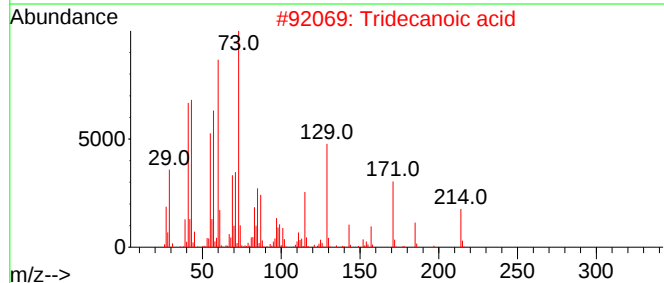
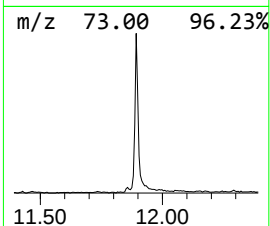
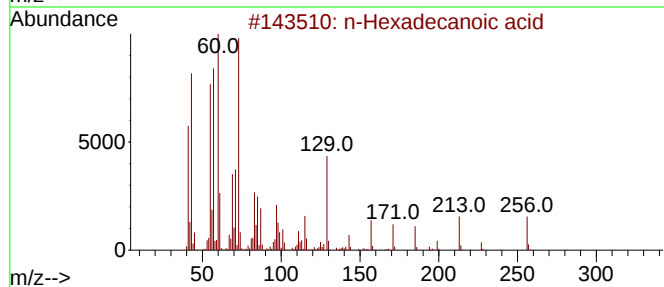
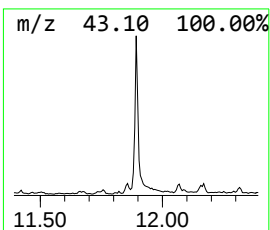
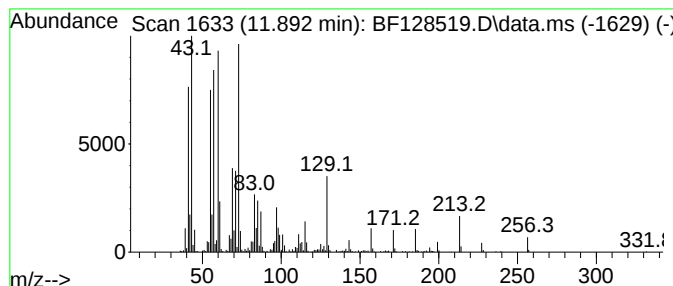
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.892 | 6.48 ng | 663110 | Phenanthrene-d10 | 11.363 |

| 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 | 94   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 87   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 78   |



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Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

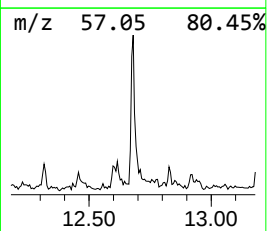
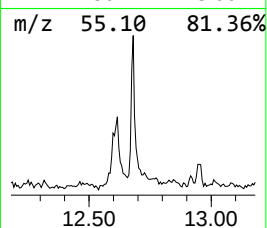
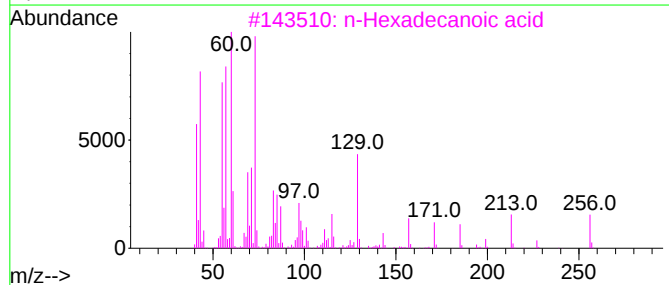
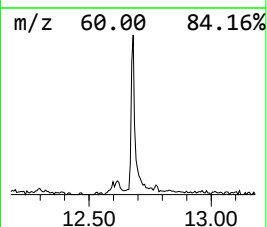
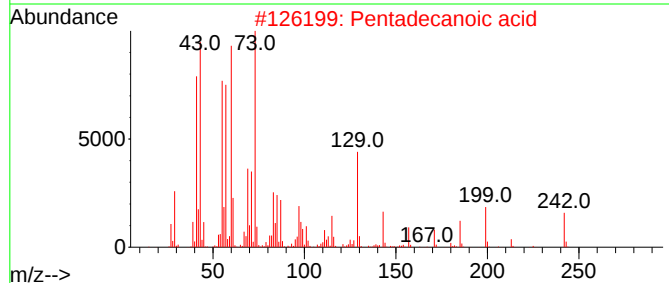
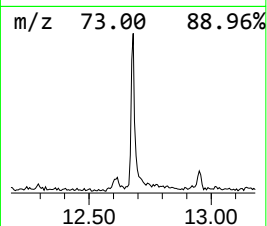
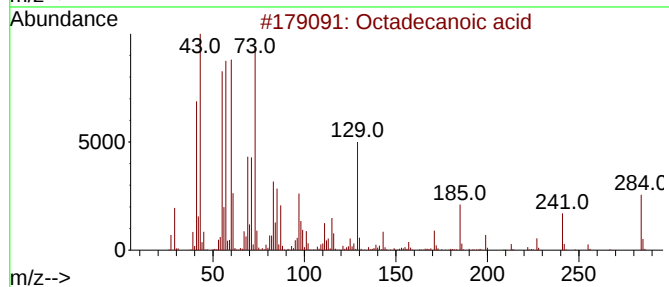
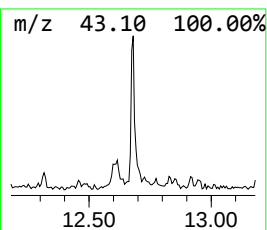
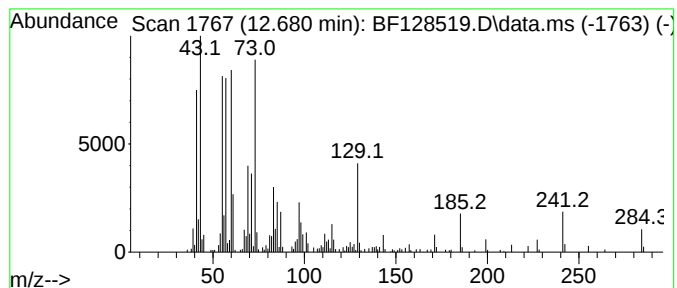
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Octadecanoic acid Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.680 | 2.55 ng | 261192 | Phenanthrene-d10 | 11.363 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 3    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 90   |
| 4    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 83   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 74   |



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Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

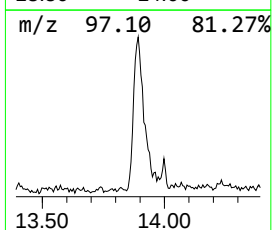
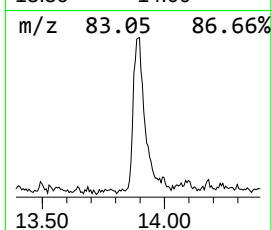
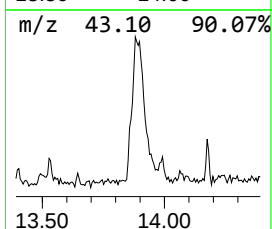
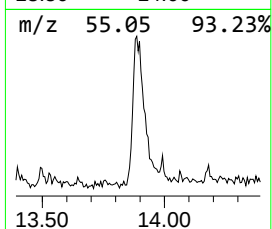
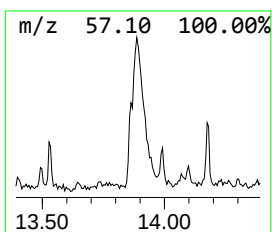
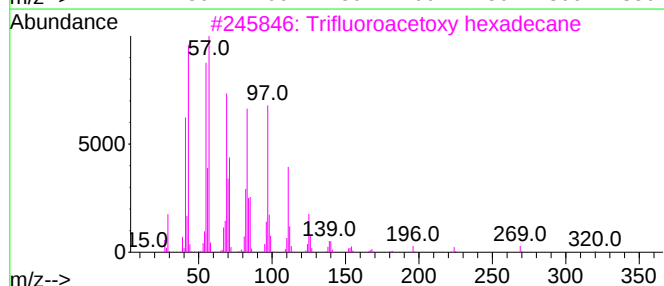
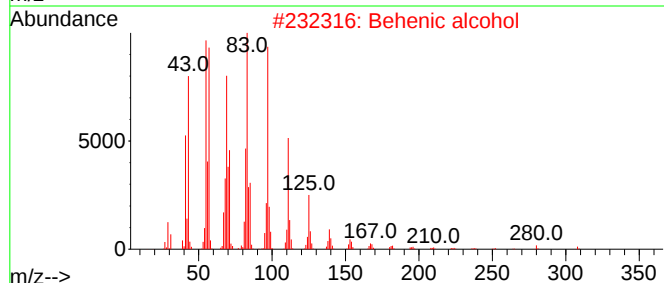
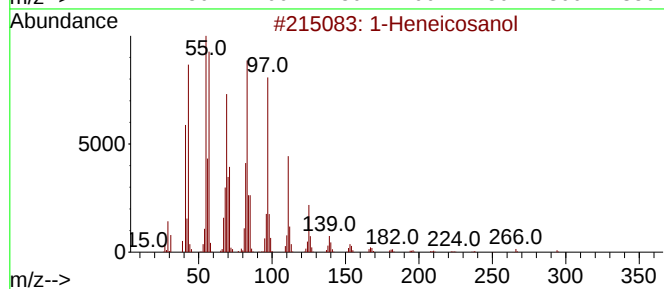
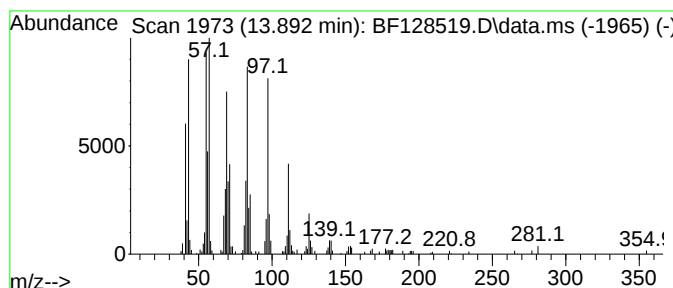
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 1-Heneicosanol Concentration Rank 3

| R.T.      | EstConc                     | Area   | Relative to ISTD | R.T.        |      |
|-----------|-----------------------------|--------|------------------|-------------|------|
| 13.892    | 6.21 ng                     | 494719 | Chrysene-d12     | 13.998      |      |
| Hit# of 5 | Tentative ID                | MW     | MolForm          | CAS#        | Qual |
| 1         | 1-Heneicosanol              | 312    | C21H44O          | 015594-90-8 | 95   |
| 2         | Behenic alcohol             | 326    | C22H46O          | 000661-19-8 | 93   |
| 3         | Trifluoroacetoxy hexadecane | 338    | C18H33F3O2       | 006222-03-3 | 93   |
| 4         | 1-Hexacosene                | 364    | C26H52           | 018835-33-1 | 93   |
| 5         | n-Tetracosanol-1            | 354    | C24H50O          | 000506-51-4 | 91   |



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ALS Vial : 7 Sample Multiplier: 1

Instrument :  
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ClientSampleId :  
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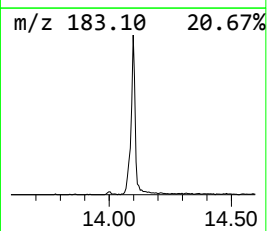
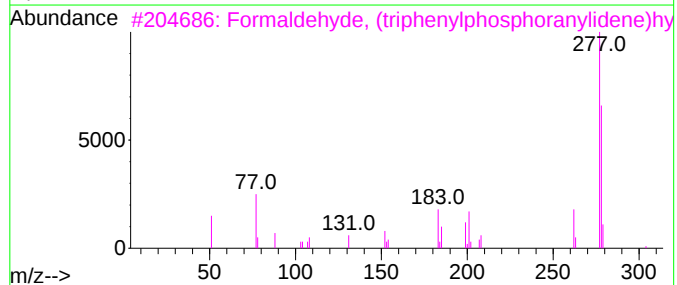
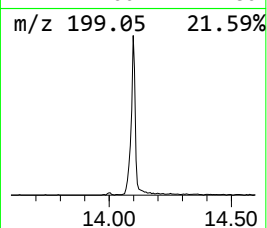
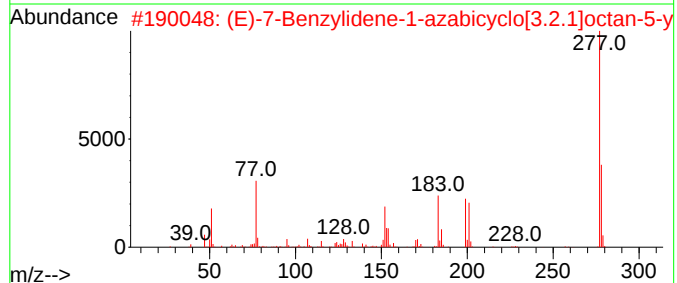
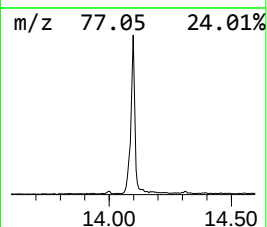
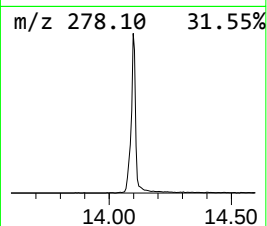
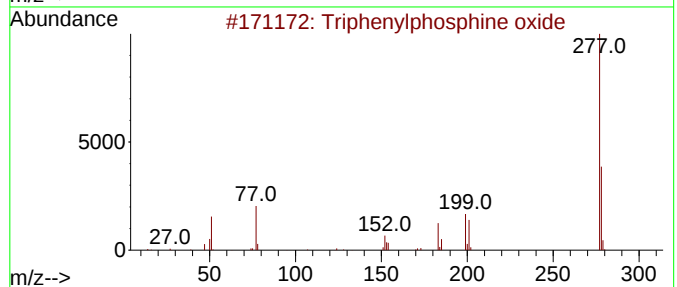
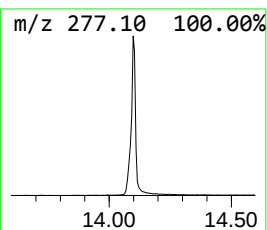
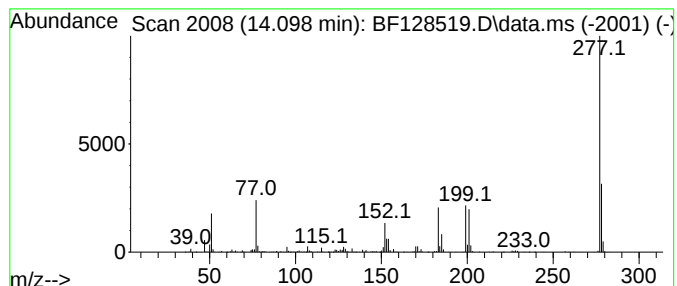
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 14.098 | 15.21 ng | 1211710 | Chrysene-d12     | 13.998 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 93   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...] | 304 | C19H17N2P  | 015990-54-2  | 64   |
| 4    |    |   | Cobalt,(.eta.<5>-2,4-cyclopentad...  | 277 | C16H15BCo  | 036682-12-9  | 35   |
| 5    |    |   | Vanadium, cycloheptatrienyl-(pen...  | 277 | C17H22V    | 1000155-20-5 | 23   |



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P024-SS004-0006-01

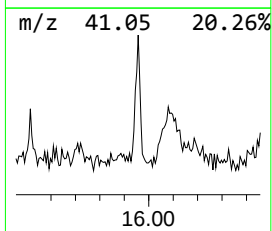
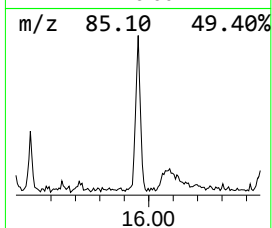
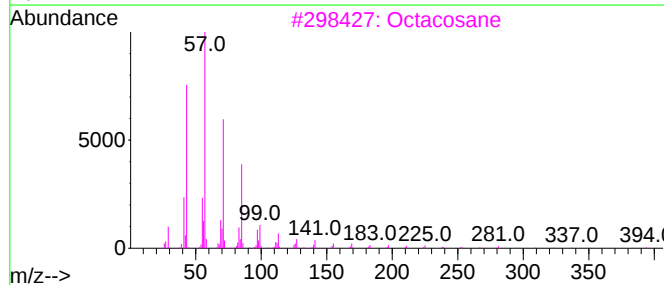
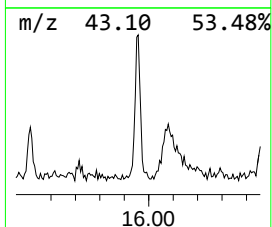
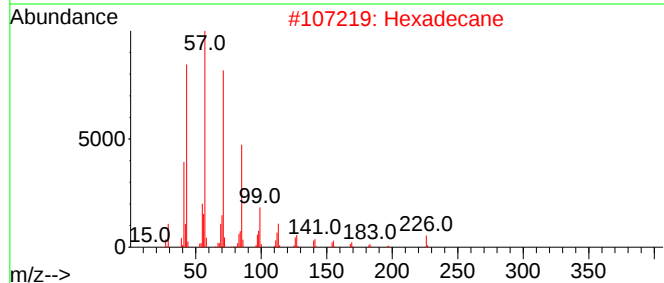
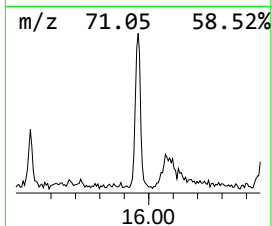
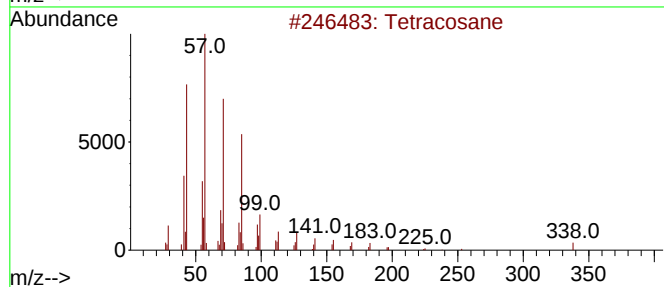
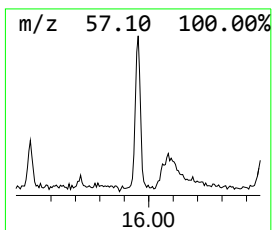
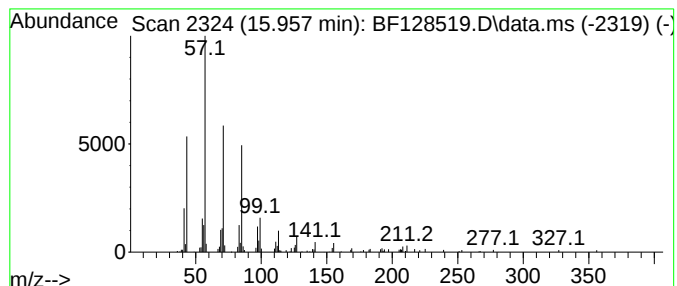
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 Tetracosane Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.957 | 2.36 ng | 146176 | Perylene-d12     | 15.463 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Tetracosane                         | 338 | C24H50    | 000646-31-1  | 87   |
| 2    |    |   | Hexadecane                          | 226 | C16H34    | 000544-76-3  | 86   |
| 3    |    |   | Octacosane                          | 394 | C28H58    | 000630-02-4  | 76   |
| 4    |    |   | Heneicosane                         | 296 | C21H44    | 000629-94-7  | 74   |
| 5    |    |   | Sulfurous acid, 2-ethylhexyl iso... | 278 | C14H30O3S | 1000309-19-0 | 72   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052722\  
Data File : BF128519.D  
Acq On : 27 May 2022 19:57  
Operator : CG\JU  
Sample : N2922-25  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

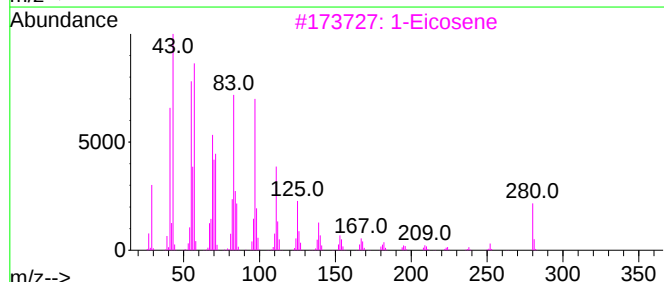
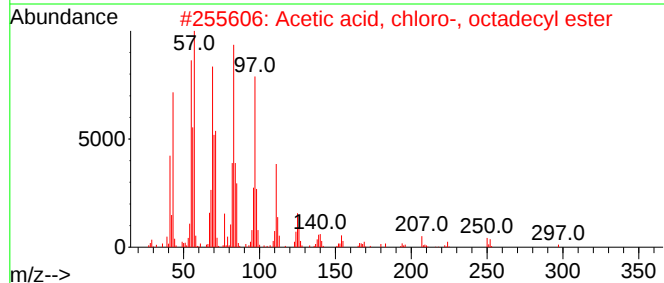
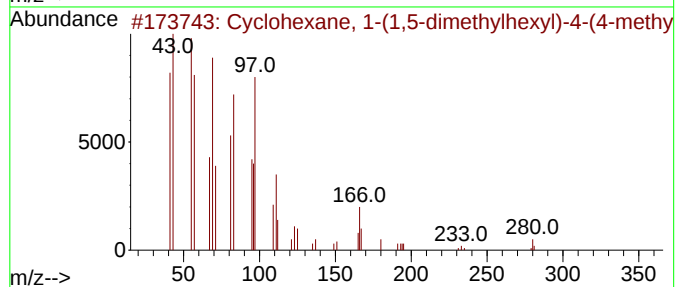
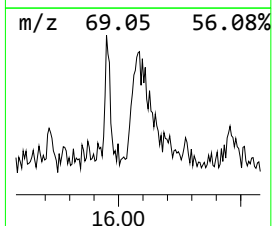
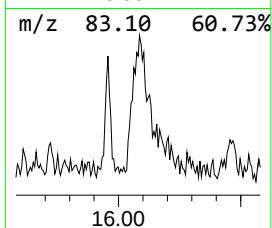
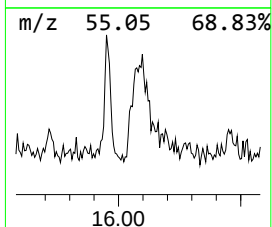
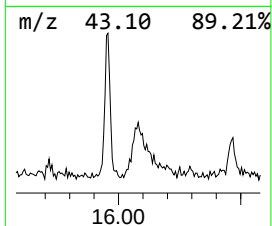
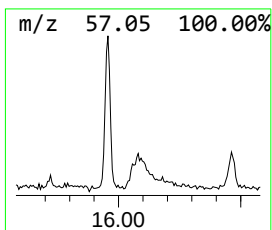
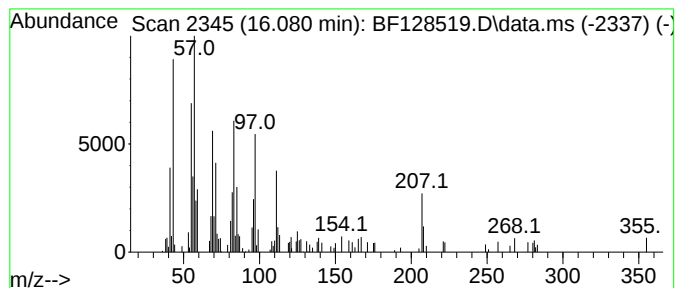
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Cyclohexane, 1-(1,5-dimethy... Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 16.080 | 2.86 ng | 177691 | Perylene-d12     | 15.463 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | Cyclohexane, 1-(1,5-dimethylhexy... | 280 | C20H40     | 056009-20-2 | 78   |
| 2    |    |   | Acetic acid, chloro-, octadecyl ... | 346 | C20H39ClO2 | 005348-82-3 | 70   |
| 3    |    |   | 1-Eicosene                          | 280 | C20H40     | 003452-07-1 | 64   |
| 4    |    |   | Pentafluoropropionic acid, hepta... | 402 | C20H35F5O2 | 959218-78-1 | 62   |
| 5    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5 | 62   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052722\  
Data File : BF128519.D  
Acq On : 27 May 2022 19:57  
Operator : CG\JU  
Sample : N2922-25  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

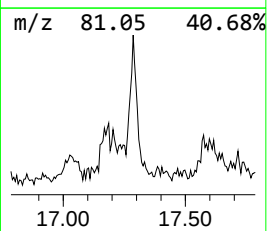
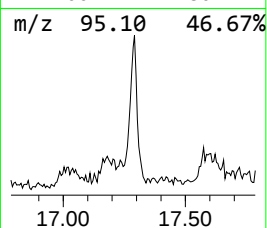
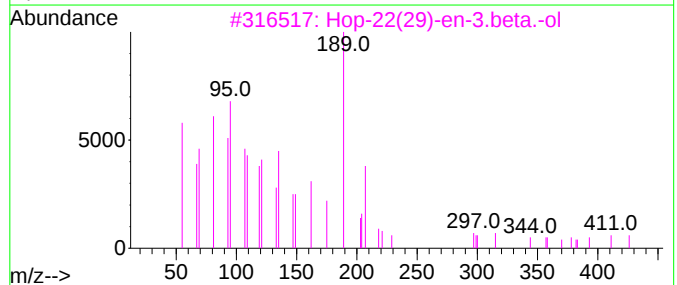
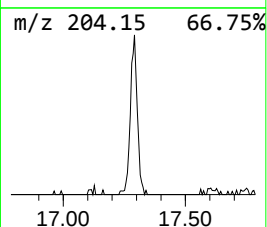
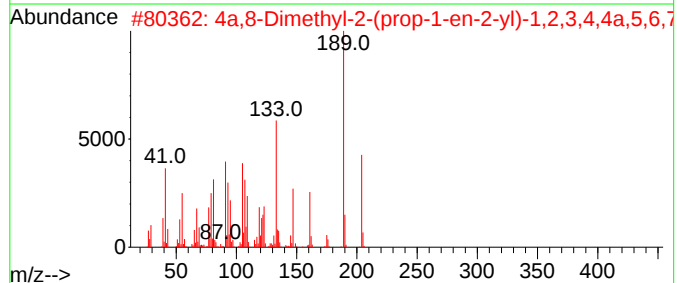
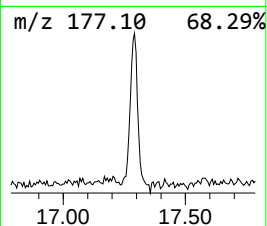
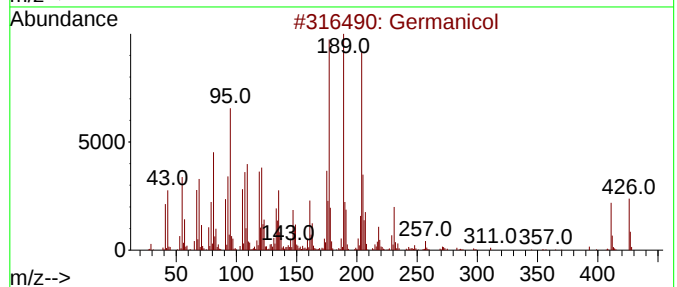
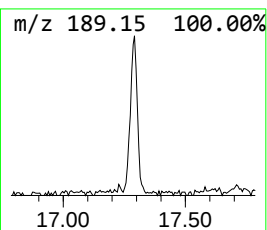
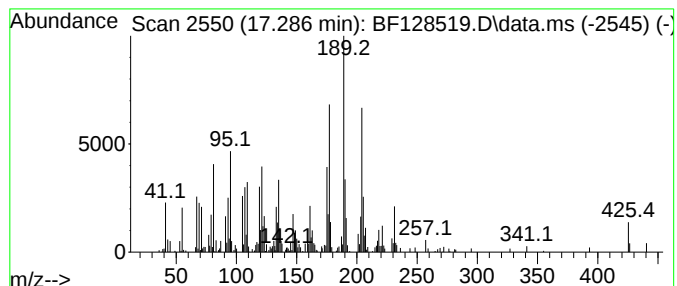
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Germanicol Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.286 | 5.48 ng | 339847 | Perylene-d12     | 15.463 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Germanicol                           | 426 | C30H50O  | 000465-02-1 | 53   |
| 2    |    |   | 4a,8-Dimethyl-2-(prop-1-en-2-yl)...  | 204 | C15H24   | 103827-22-1 | 38   |
| 3    |    |   | Hop-22(29)-en-3.beta.-ol             | 426 | C30H50O  | 058801-23-3 | 35   |
| 4    |    |   | 1,2,4,8-Tetramethylbicyclo[6.3.0]... | 204 | C15H24   | 137235-51-9 | 30   |
| 5    |    |   | 3,4-Dihydrocoumarin, 4,4,7,8-tet...  | 204 | C13H16O2 | 040614-36-6 | 27   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052722\  
Data File : BF128519.D  
Acq On : 27 May 2022 19:57  
Operator : CG\JU  
Sample : N2922-25  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

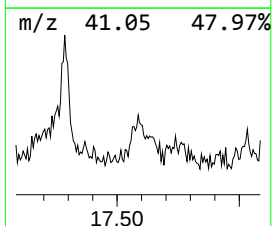
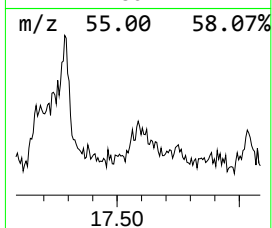
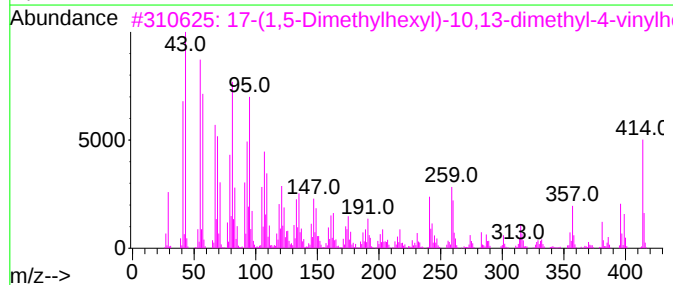
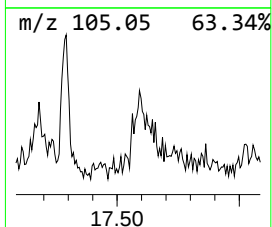
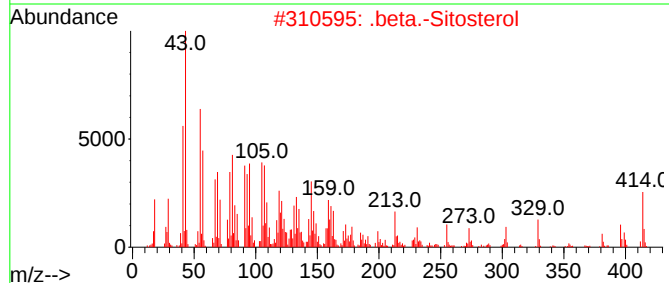
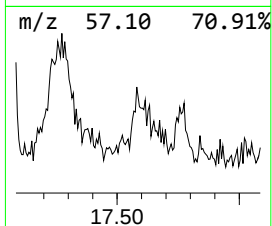
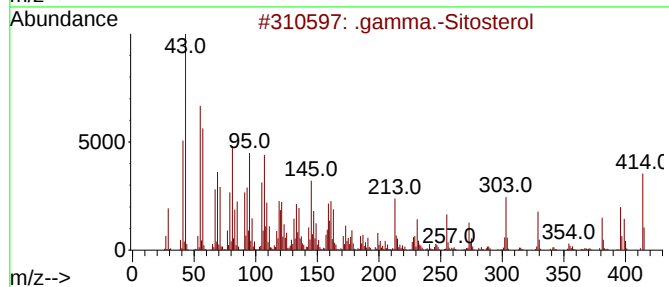
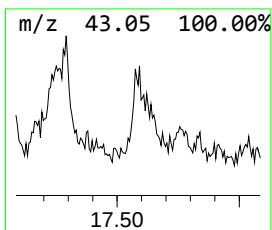
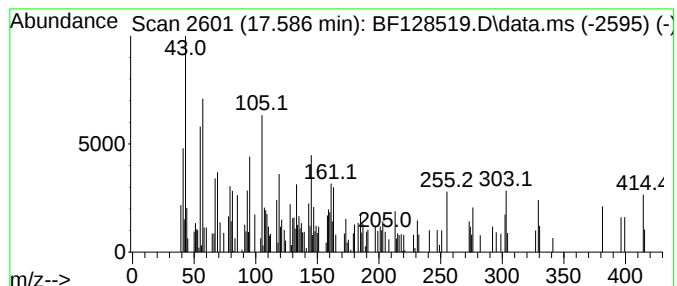
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 .gamma.-Sitosterol Concentration Rank 8

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.586 | 2.19 ng | 135804 | Perylene-d12     | 15.463 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|------|-------------------------------------|-----|----------|--------------|------|
| 1    |      | .gamma.-Sitosterol                  | 414 | C29H50O  | 000083-47-6  | 91   |
| 2    |      | .beta.-Sitosterol                   | 414 | C29H50O  | 000083-46-5  | 60   |
| 3    |      | 17-(1,5-Dimethylhexyl)-10,13-dim... | 414 | C29H50O  | 1000210-86-9 | 35   |
| 4    |      | Cholest-5-ene, 3-ethoxy-, (3.bet... | 414 | C29H50O  | 000986-19-6  | 25   |
| 5    |      | .beta.-Sitosterol acetate           | 456 | C31H52O2 | 000915-05-9  | 16   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF052722\  
Data File : BF128519.D  
Acq On : 27 May 2022 19:57  
Operator : CG\JU  
Sample : N2922-25  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
P024-SS004-0006-01

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF052622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| n-Hexadecanoic ... | 11.892 | 6.5     | ng    | 663110   | 4                     | 11.363 | 2046370 | 20.0 |
| Octadecanoic acid  | 12.680 | 2.5     | ng    | 261192   | 4                     | 11.363 | 2046370 | 20.0 |
| 1-Heneicosanol     | 13.892 | 6.2     | ng    | 494719   | 5                     | 13.998 | 1593780 | 20.0 |
| Triphenylphosph... | 14.098 | 15.2    | ng    | 1211710  | 5                     | 13.998 | 1593780 | 20.0 |
| Tetracosane        | 15.957 | 2.4     | ng    | 146176   | 6                     | 15.463 | 1240750 | 20.0 |
| Cyclohexane, 1-... | 16.080 | 2.9     | ng    | 177691   | 6                     | 15.463 | 1240750 | 20.0 |
| Germanicol         | 17.286 | 5.5     | ng    | 339847   | 6                     | 15.463 | 1240750 | 20.0 |
| .gamma.-Sitosterol | 17.586 | 2.2     | ng    | 135804   | 6                     | 15.463 | 1240750 | 20.0 |