

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071923\  
 Data File : BF134358.D  
 Acq On : 19 Jul 2023 14:45  
 Operator : CG\JU  
 Sample : 03597-18  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 RB-50-(2-5)

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134358.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         | 2.152       | 5             | 11          | 23           | rVB      | 388008         | 509101        | 26.14%          | 3.938%        |
| 2         | 5.093       | 506           | 511         | 518          | rVB      | 23297          | 29015         | 1.49%           | 0.224%        |
| 3         | 5.481       | 573           | 577         | 593          | rBV      | 1680382        | 1528877       | 78.49%          | 11.827%       |
| 4         | 6.481       | 742           | 747         | 750          | rBV      | 1574025        | 1537735       | 78.95%          | 11.896%       |
| 5         | 6.675       | 774           | 780         | 788          | rBV2     | 14386          | 25937         | 1.33%           | 0.201%        |
| 6         | 6.834       | 804           | 807         | 815          | rBV      | 490484         | 449177        | 23.06%          | 3.475%        |
| 7         | 7.404       | 899           | 904         | 907          | rBV      | 1042765        | 1015438       | 52.13%          | 7.855%        |
| 8         | 8.116       | 1021          | 1025        | 1028         | rBV      | 735956         | 559686        | 28.73%          | 4.330%        |
| 9         | 9.192       | 1204          | 1208        | 1211         | rBV      | 2424207        | 1947768       | 100.00%         | 15.068%       |
| 10        | 9.304       | 1224          | 1227        | 1232         | rVB      | 25919          | 24107         | 1.24%           | 0.186%        |
| 11        | 9.875       | 1320          | 1324        | 1327         | rBV      | 748438         | 595320        | 30.56%          | 4.605%        |
| 12        | 10.669      | 1455          | 1459        | 1470         | rBV      | 1333616        | 1152403       | 59.17%          | 8.915%        |
| 13        | 11.369      | 1574          | 1578        | 1585         | rBV      | 675748         | 550709        | 28.27%          | 4.260%        |
| 14        | 11.898      | 1662          | 1668        | 1686         | rBV      | 279502         | 327271        | 16.80%          | 2.532%        |
| 15        | 12.051      | 1690          | 1694        | 1701         | rVV5     | 23840          | 44091         | 2.26%           | 0.341%        |
| 16        | 12.592      | 1781          | 1786        | 1788         | rBV      | 28062          | 32590         | 1.67%           | 0.252%        |
| 17        | 12.686      | 1798          | 1802        | 1811         | rBV      | 72109          | 85509         | 4.39%           | 0.661%        |
| 18        | 12.968      | 1845          | 1850        | 1853         | rBV      | 1655912        | 1496298       | 76.82%          | 11.575%       |
| 19        | 13.892      | 1997          | 2007        | 2017         | rBV      | 82635          | 189123        | 9.71%           | 1.463%        |
| 20        | 14.033      | 2027          | 2031        | 2040         | rVB      | 408829         | 403045        | 20.69%          | 3.118%        |
| 21        | 14.121      | 2042          | 2046        | 2052         | rVB      | 79899          | 88126         | 4.52%           | 0.682%        |
| 22        | 15.539      | 2282          | 2287        | 2295         | rVB      | 247773         | 335596        | 17.23%          | 2.596%        |

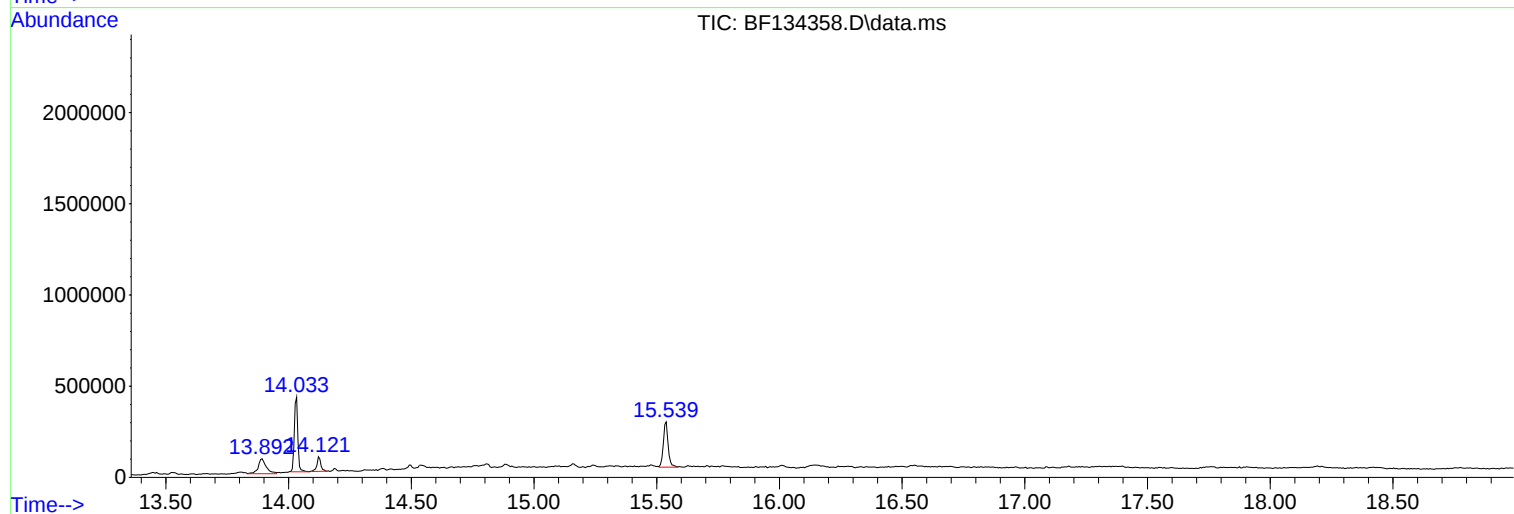
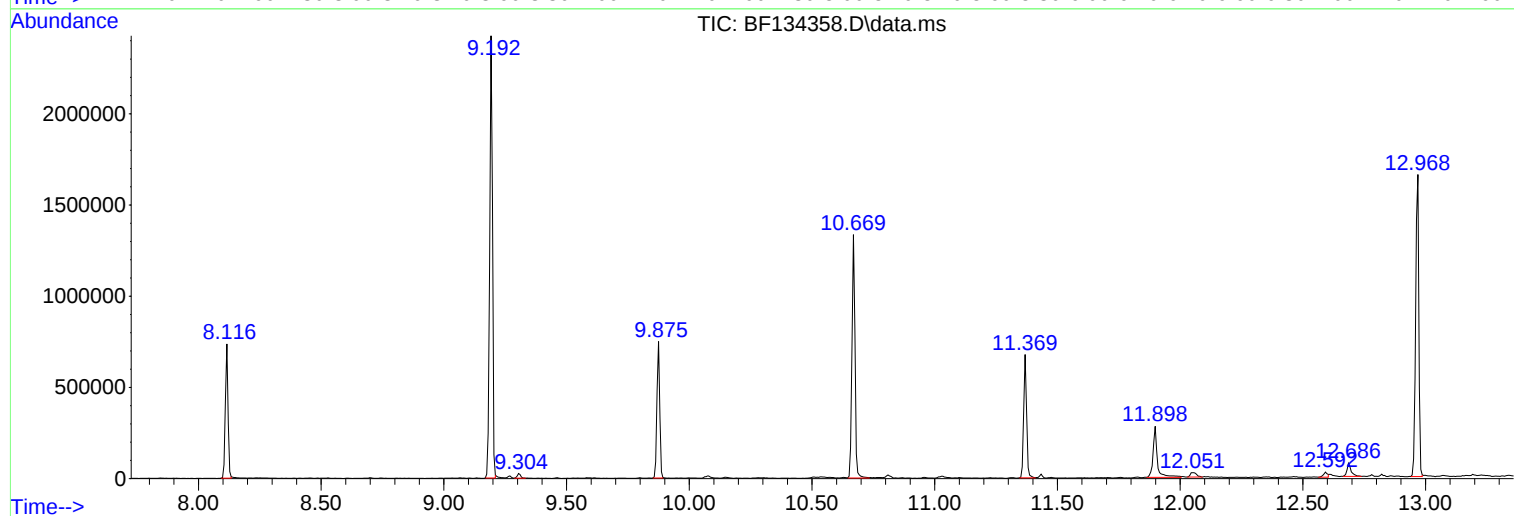
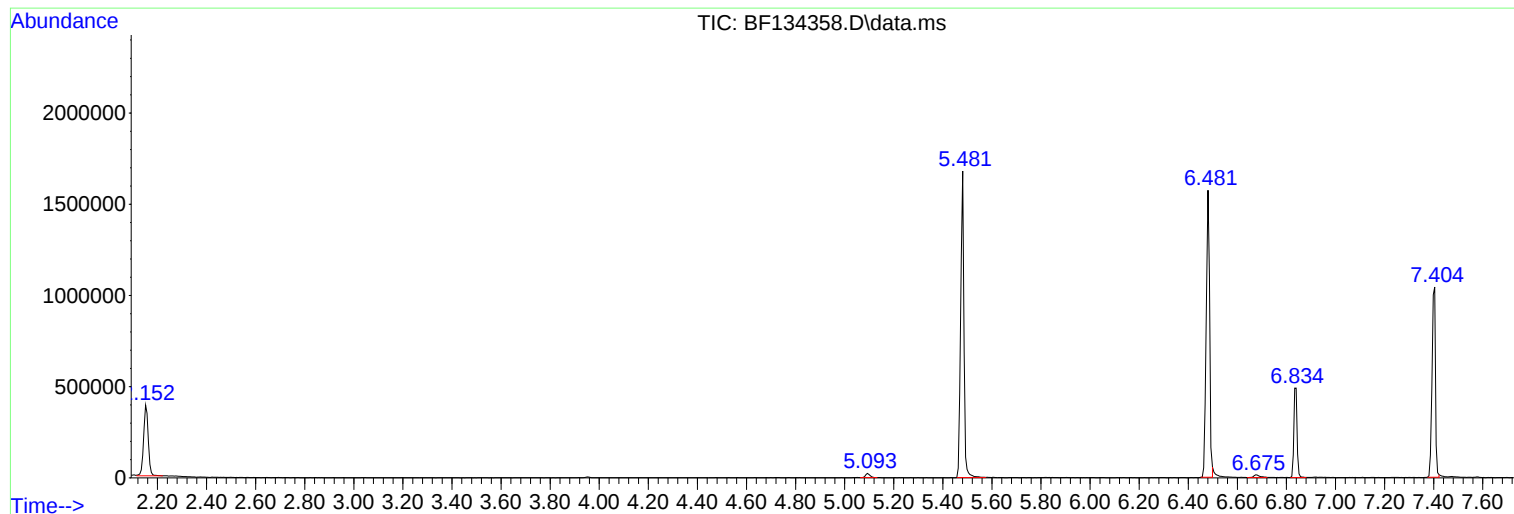
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Instrument :  
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ClientSampleId :  
RB-50-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.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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RB-50-(2-5)

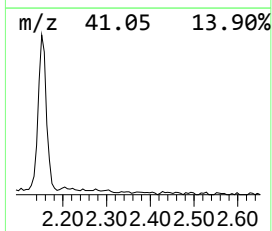
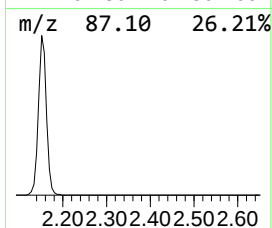
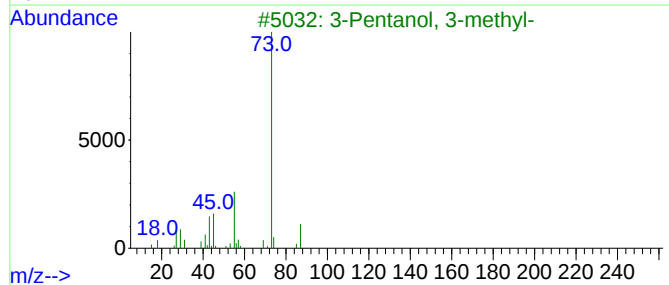
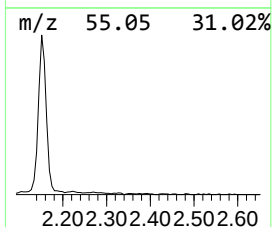
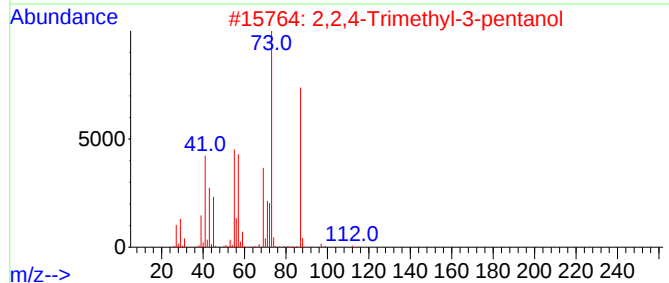
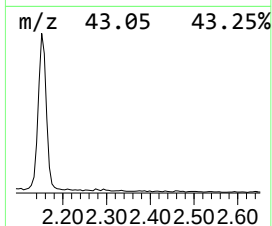
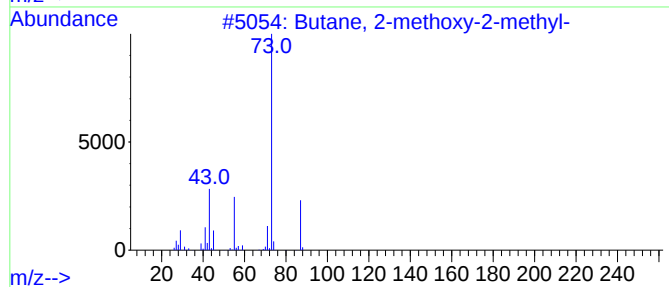
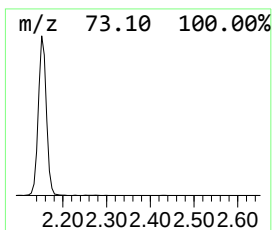
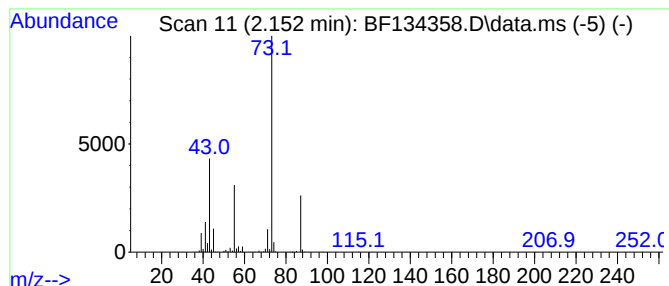
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 2.152 | 22.67 ng | 509101 | 1,4-Dichlorobenzene-d4 | 6.839 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 40   |
| 3    |    |   | 3-Pentanol, 3-methyl-       | 102 | C6H14O  | 000077-74-7 | 38   |
| 4    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 38   |
| 5    |    |   | 3-Pentanol, 2,4-dimethyl-   | 116 | C7H16O  | 000600-36-2 | 37   |



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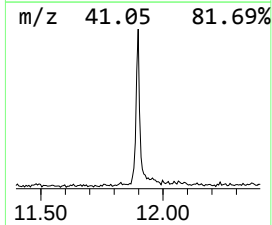
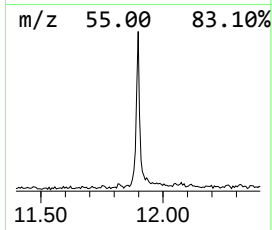
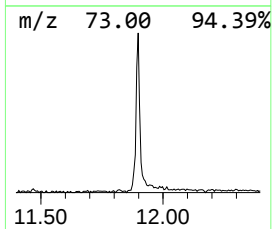
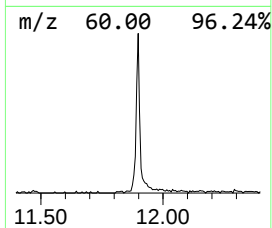
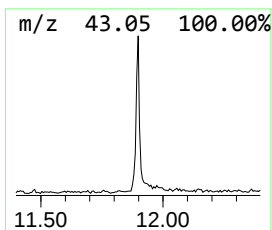
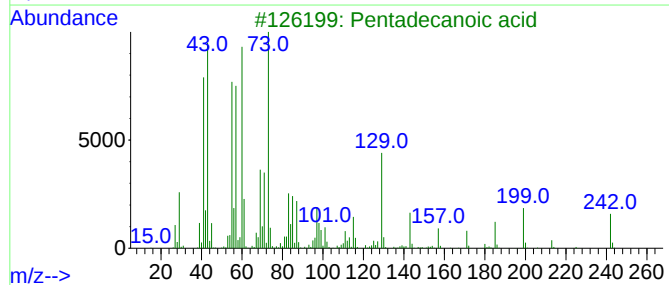
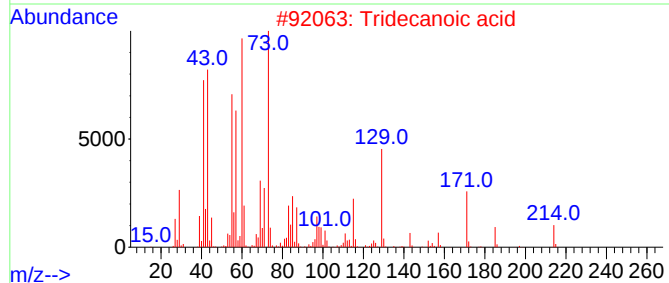
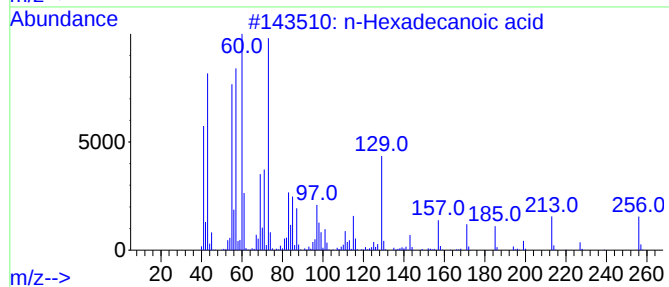
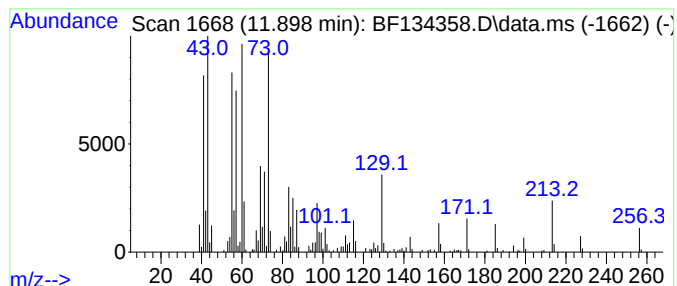
Instrument :  
BNA\_F  
ClientSampleId :  
RB-50-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.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 n-Hexadecanoic acid Concentration Rank 2

| R.T.      | EstConc             | Area   | Relative to ISTD |          | R.T.        |      |
|-----------|---------------------|--------|------------------|----------|-------------|------|
| 11.898    | 11.89 ng            | 327271 | Phenanthrene-d10 |          | 11.369      |      |
| Hit# of 5 | Tentative ID        |        | MW               | MolForm  | CAS#        | Qual |
| 1         | n-Hexadecanoic acid |        | 256              | C16H32O2 | 000057-10-3 | 98   |
| 2         | Tridecanoic acid    |        | 214              | C13H26O2 | 000638-53-9 | 94   |
| 3         | Pentadecanoic acid  |        | 242              | C15H30O2 | 001002-84-2 | 91   |
| 4         | Tetradecanoic acid  |        | 228              | C14H28O2 | 000544-63-8 | 72   |
| 5         | Dodecanoic acid     |        | 200              | C12H24O2 | 000143-07-7 | 70   |



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Sample : 03597-18  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RB-50-(2-5)

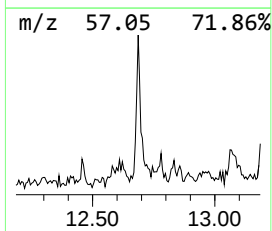
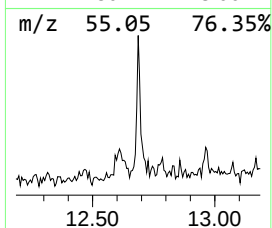
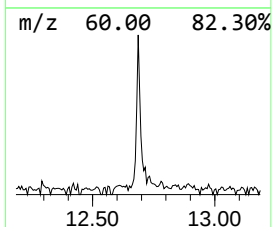
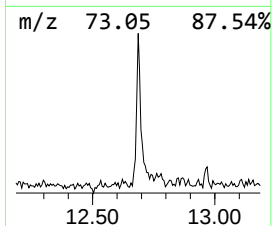
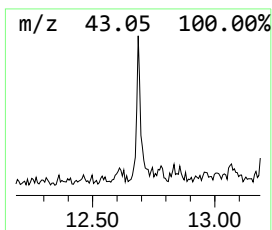
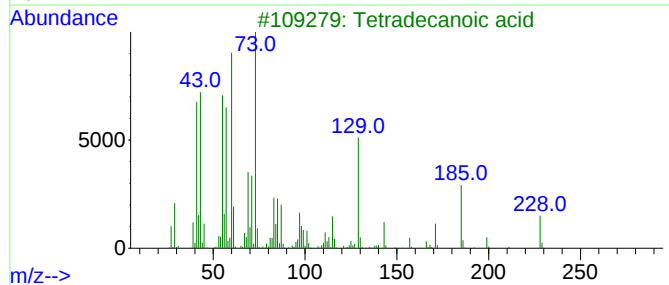
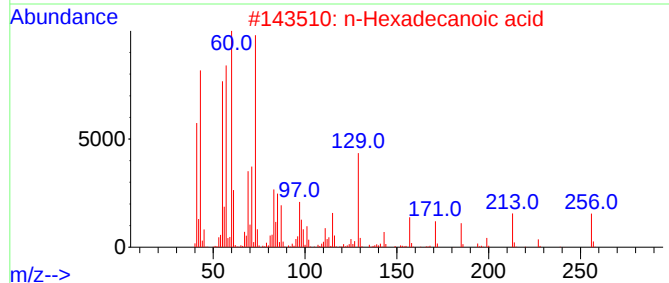
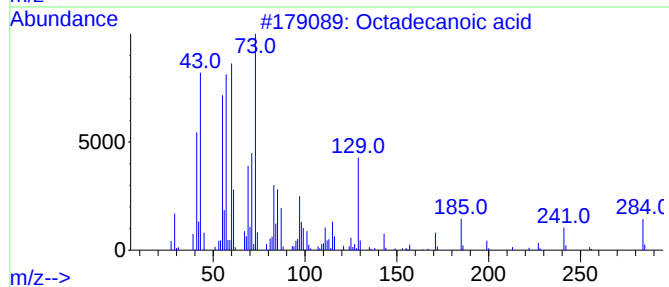
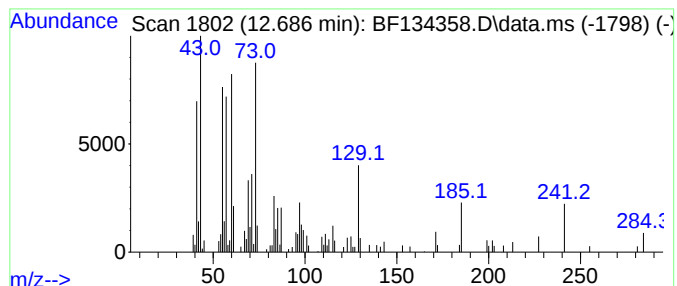
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 12.686 | 3.11 ng | 85509 | Phenanthrene-d10 | 11.369 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 95   |
| 2    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 87   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 80   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 64   |



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ClientSampleId :  
RB-50-(2-5)

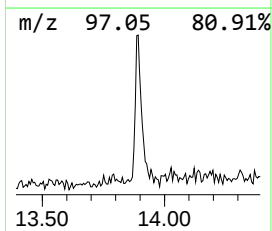
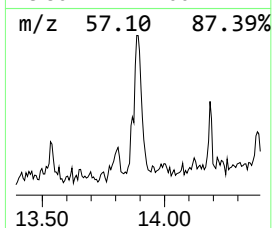
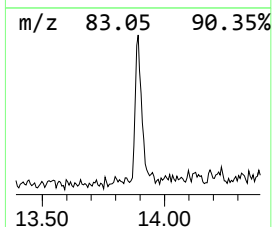
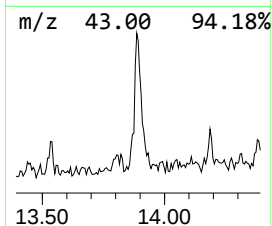
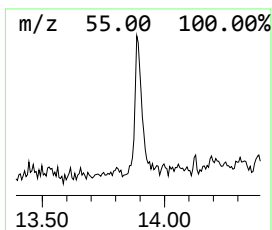
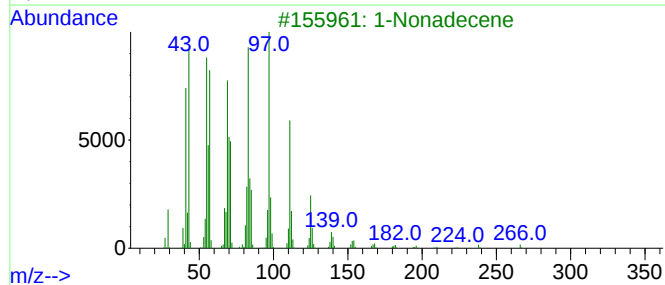
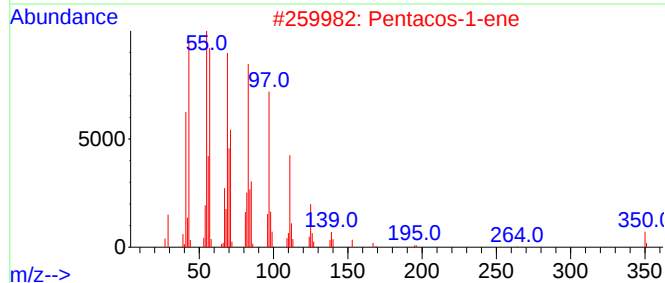
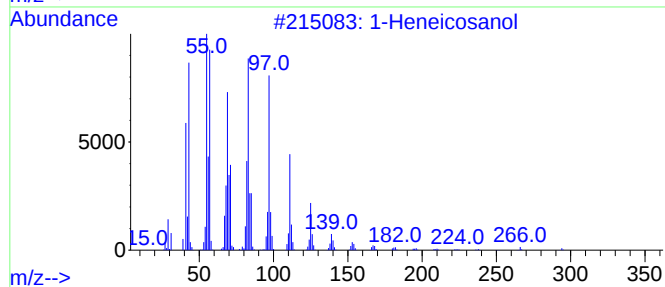
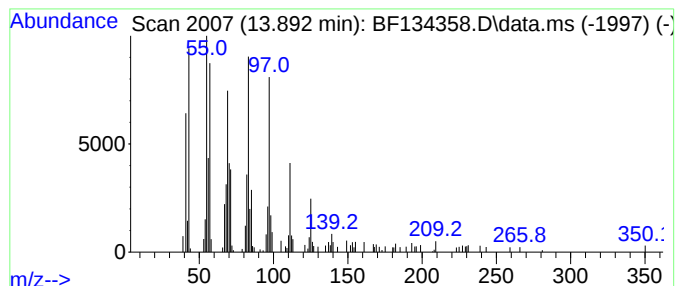
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Peak Number 4 1-Heneicosanol Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.892 | 9.38 ng | 189123 | Chrysene-d12     | 14.033 |

| Hit# | of 5 | Tentative ID     | MW  | MolForm | CAS#        | Qual |
|------|------|------------------|-----|---------|-------------|------|
| 1    |      | 1-Heneicosanol   | 312 | C21H44O | 015594-90-8 | 94   |
| 2    |      | Pentacos-1-ene   | 350 | C25H50  | 016980-85-1 | 93   |
| 3    |      | 1-Nonadecene     | 266 | C19H38  | 018435-45-5 | 93   |
| 4    |      | 1-Tetracosene    | 336 | C24H48  | 010192-32-2 | 91   |
| 5    |      | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 87   |



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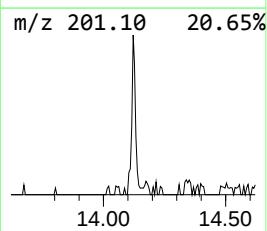
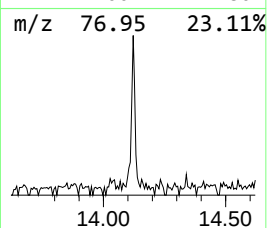
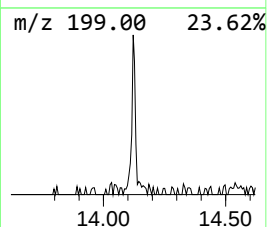
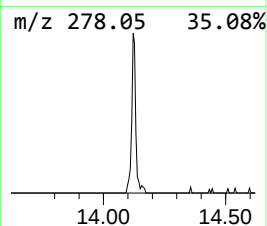
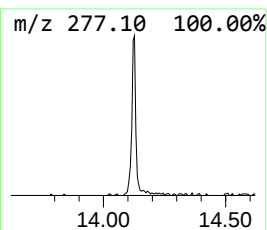
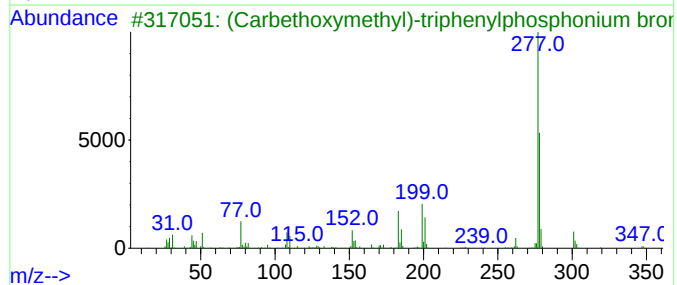
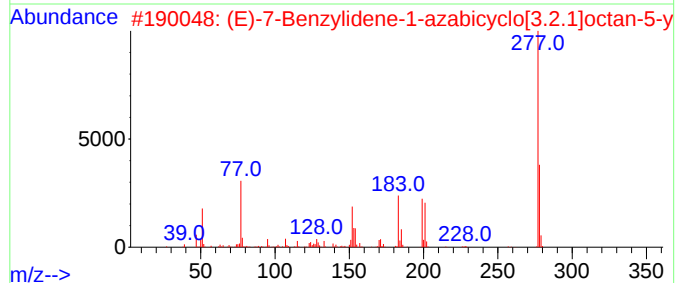
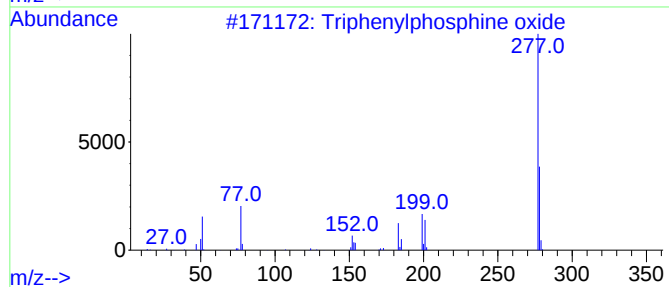
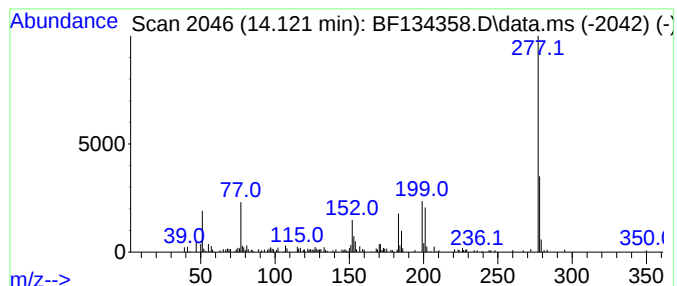
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TIC Integration Parameters: LSCINT.P

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Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.121 | 4.37 ng | 88126 | Chrysene-d12     | 14.033 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 96   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S  | 1000483-83-4 | 90   |
| 3    |    |   | (Carbethoxymethyl)-triphenylphos...  | 428 | C22H22BrO2P | 001530-45-6  | 50   |
| 4    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 50   |
| 5    |    |   | 3-(3,4-Dichlorophenyl)-2-thioxo-...  | 277 | C9H5Cl2NOS2 | 017046-34-3  | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF071923\  
Data File : BF134358.D  
Acq On : 19 Jul 2023 14:45  
Operator : CG\JU  
Sample : 03597-18  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
RB-50-(2-5)

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062623.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 |
| Butane, 2-metho... | 2.152  | 22.7    | ng    | 509101   | 1                     | 6.839  | 449177 | 20.0 |
| n-Hexadecanoic ... | 11.898 | 11.9    | ng    | 327271   | 4                     | 11.369 | 550709 | 20.0 |
| Octadecanoic acid  | 12.686 | 3.1     | ng    | 85509    | 4                     | 11.369 | 550709 | 20.0 |
| 1-Heneicosanol     | 13.892 | 9.4     | ng    | 189123   | 5                     | 14.033 | 403045 | 20.0 |
| Triphenylphosph... | 14.121 | 4.4     | ng    | 88126    | 5                     | 14.033 | 403045 | 20.0 |