

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP090922\  
 Data File : BP011670.D  
 Acq On : 09 Sep 2022 19:06  
 Operator : CG/JU  
 Sample : N4549-20  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 MW-64

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\_P\Methods\8270E-BP090222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011670.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         | 3.017       | 3             | 5           | 13           | rVB      | 1260461        | 1570832       | 2.62%           | 0.945%        |
| 2         | 3.093       | 13            | 18          | 44           | rVB      | 11983520       | 15315127      | 25.53%          | 9.217%        |
| 3         | 5.516       | 422           | 430         | 440          | rBV      | 3393830        | 5016764       | 8.36%           | 3.019%        |
| 4         | 7.110       | 694           | 701         | 716          | rVB      | 1975876        | 3289577       | 5.48%           | 1.980%        |
| 5         | 7.957       | 838           | 845         | 853          | rBV      | 1347518        | 2192987       | 3.66%           | 1.320%        |
| 6         | 9.128       | 1033          | 1044        | 1053         | rBV      | 4270306        | 7024110       | 11.71%          | 4.227%        |
| 7         | 10.775      | 1316          | 1324        | 1332         | rBV      | 1817705        | 3092578       | 5.16%           | 1.861%        |
| 8         | 13.228      | 1734          | 1741        | 1755         | rVB      | 11479258       | 17104388      | 28.51%          | 10.294%       |
| 9         | 14.598      | 1967          | 1974        | 1989         | rBV      | 2722499        | 3994662       | 6.66%           | 2.404%        |
| 10        | 16.086      | 2220          | 2227        | 2249         | rBV      | 8088375        | 12052688      | 20.09%          | 7.254%        |
| 11        | 17.357      | 2436          | 2443        | 2455         | rVB      | 3242916        | 4676170       | 7.80%           | 2.814%        |
| 12        | 18.239      | 2588          | 2593        | 2602         | rBV      | 515693         | 919666        | 1.53%           | 0.553%        |
| 13        | 19.469      | 2797          | 2802        | 2816         | rBV      | 358379         | 698559        | 1.16%           | 0.420%        |
| 14        | 19.904      | 2871          | 2876        | 2882         | rBV      | 14621015       | 18045760      | 30.08%          | 10.860%       |
| 15        | 21.433      | 3131          | 3136        | 3142         | rBV      | 4185743        | 5351060       | 8.92%           | 3.220%        |
| 16        | 21.568      | 3152          | 3159        | 3190         | rBV      | 34003534       | 59984749      | 100.00%         | 36.101%       |
| 17        | 23.904      | 3549          | 3556        | 3566         | rVB      | 2904994        | 5830569       | 9.72%           | 3.509%        |

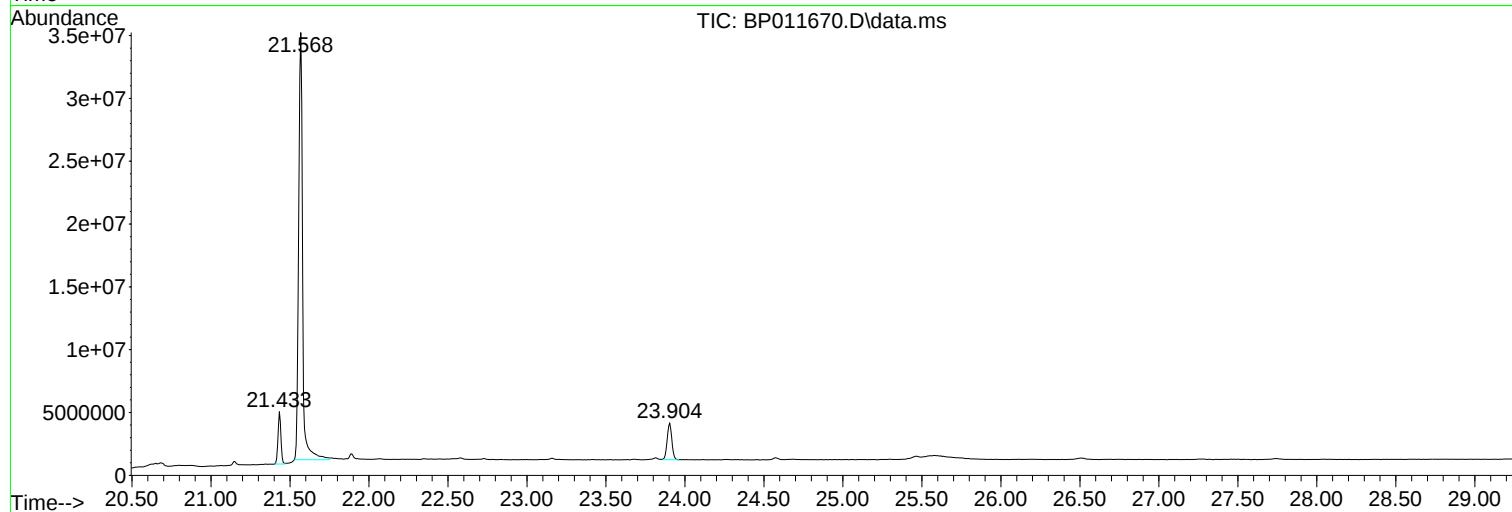
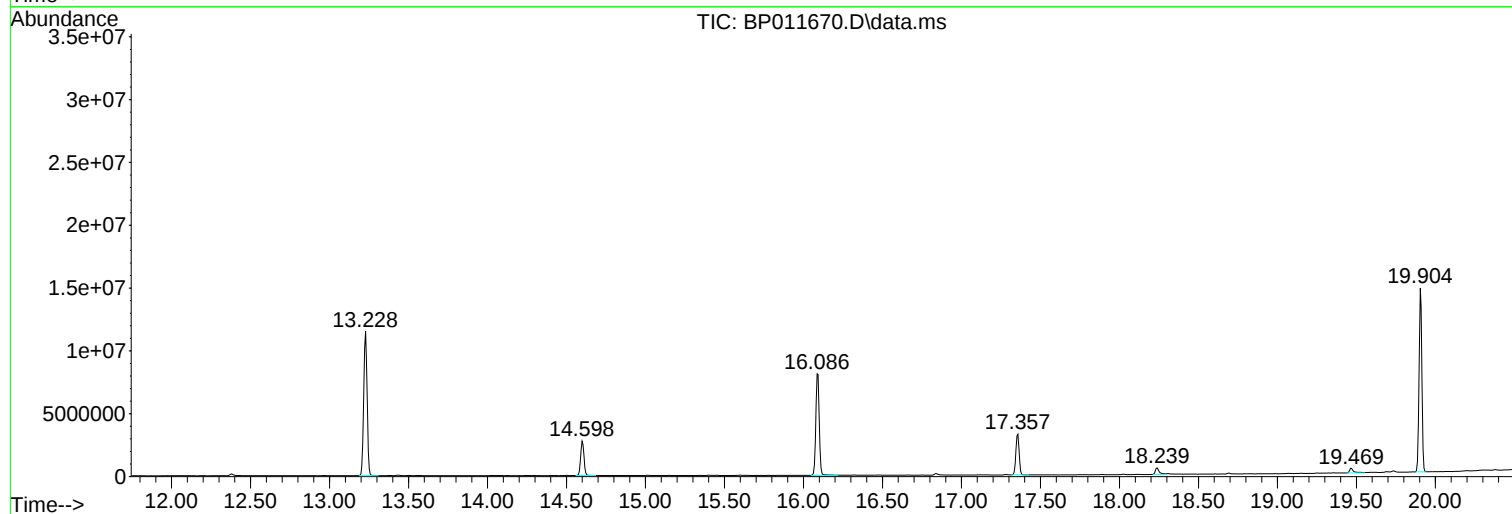
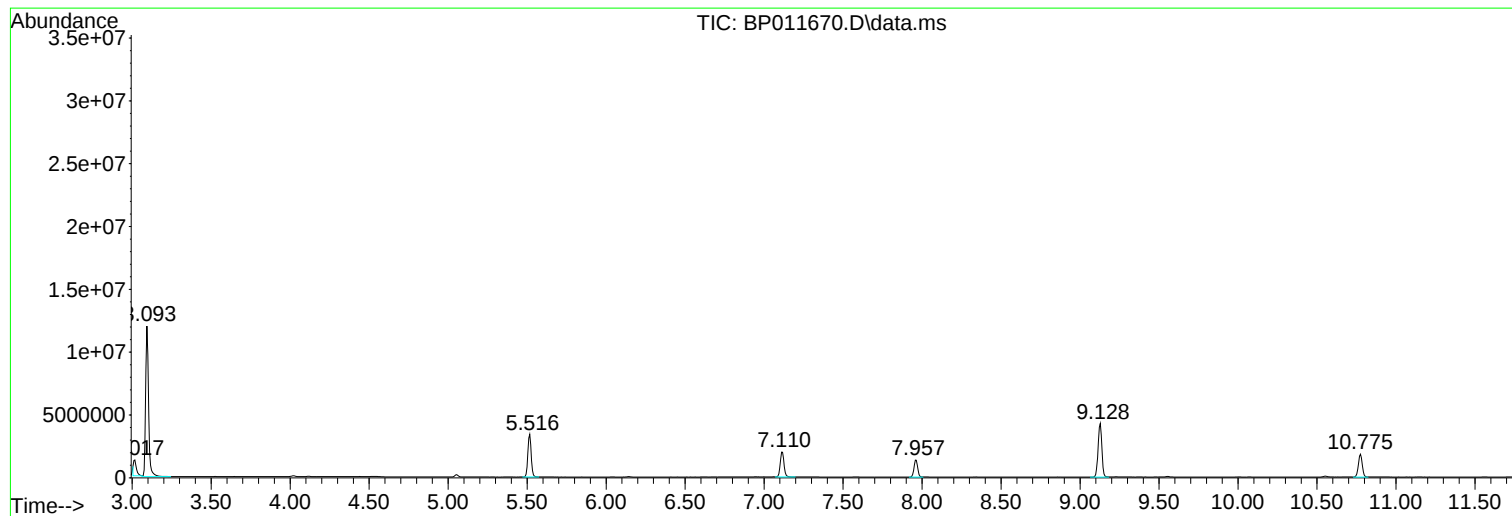
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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
MW-64

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP090222.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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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

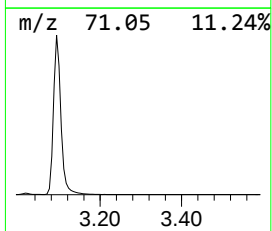
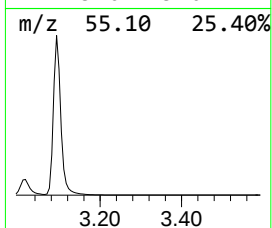
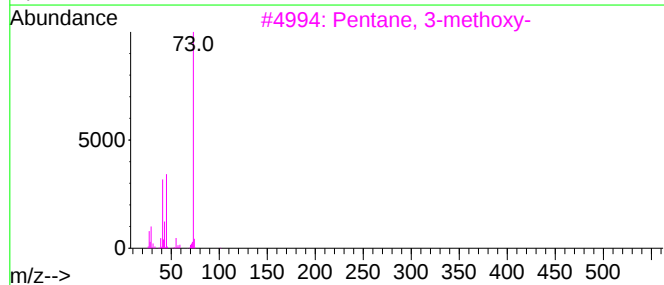
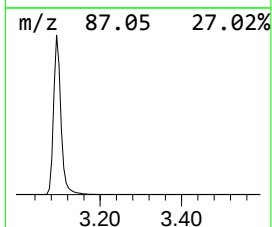
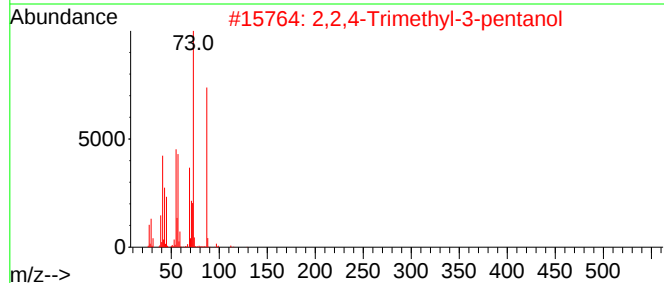
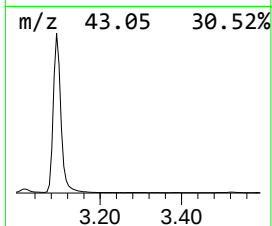
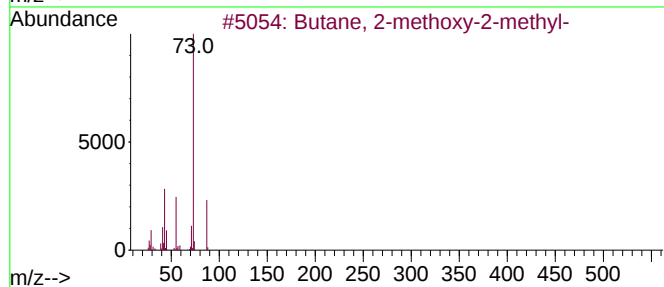
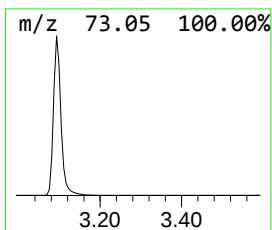
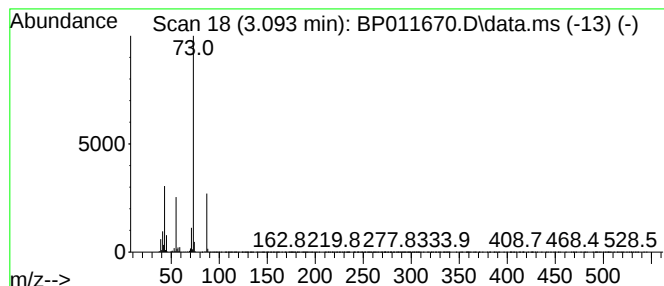
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc   | Area     | Relative to ISTD       | R.T.  |
|-------|-----------|----------|------------------------|-------|
| 3.093 | 139.67 ng | 15315100 | 1,4-Dichlorobenzene-d4 | 7.963 |

| 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 | 43   |
| 3    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 4    |    |   | 1,3-Dioxolane, 2-methyl-    | 88  | C4H8O2  | 000497-26-7 | 9    |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 9    |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP090222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

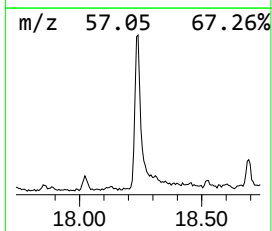
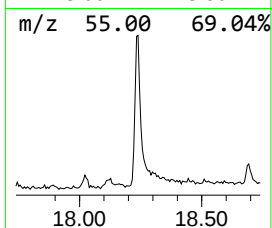
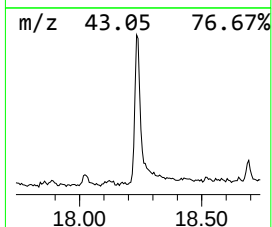
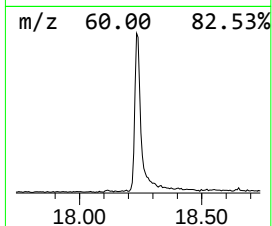
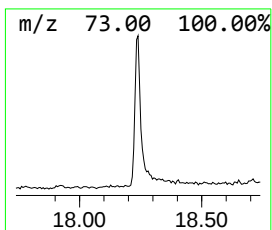
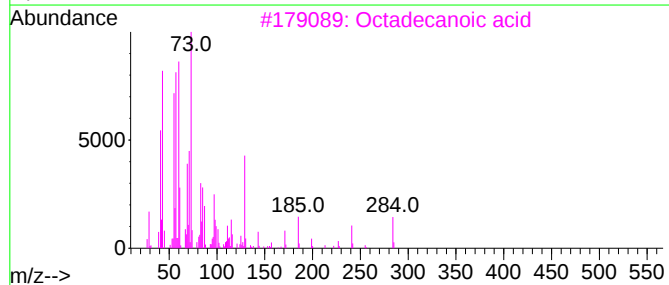
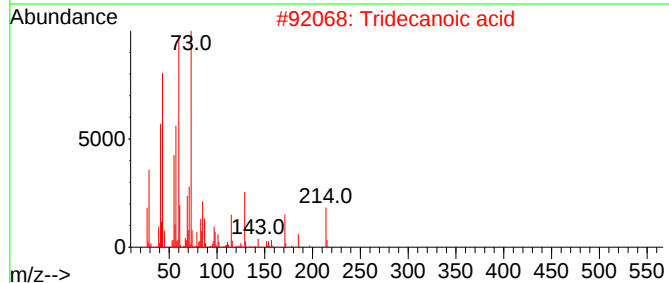
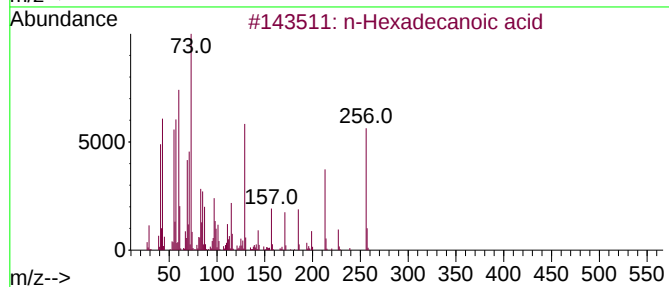
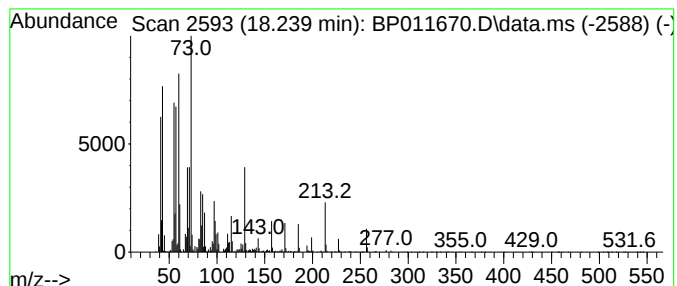
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.239 | 3.93 ng | 919666 | Phenanthrene-d10 | 17.357 |

| 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 | 93   |
| 3    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 93   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 90   |



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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
MW-64

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP090222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

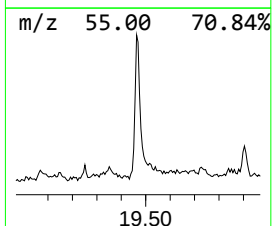
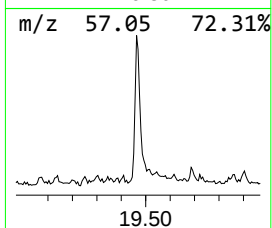
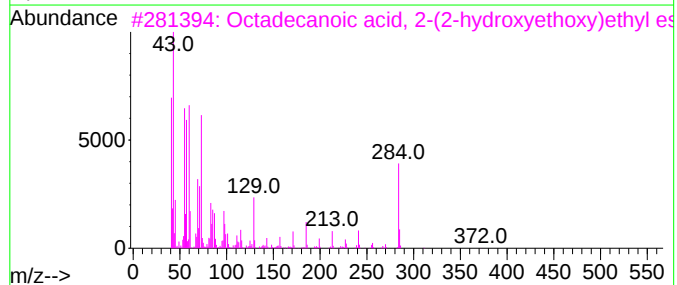
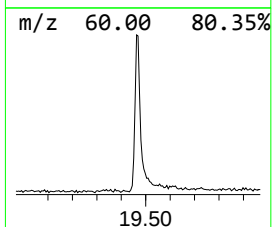
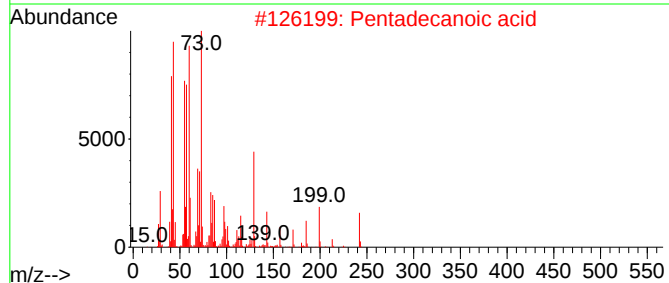
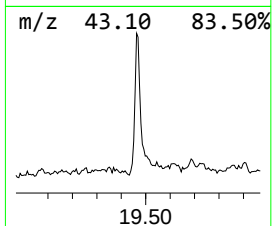
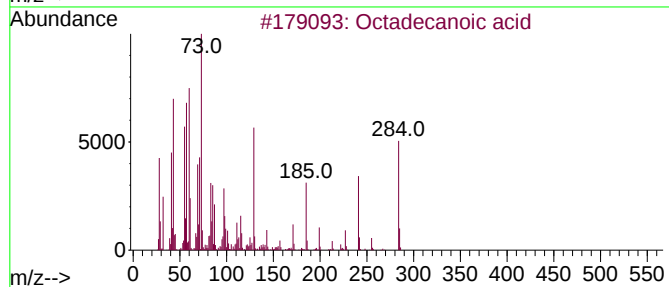
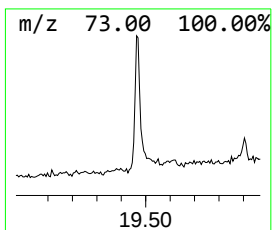
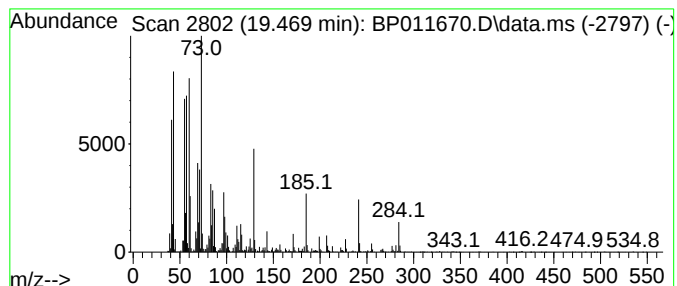
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.469 | 2.61 ng | 698559 | Chrysene-d12     | 21.433 |

| 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    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 90   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 5    |    |   | n-Decanoic acid                     | 172 | C10H20O2 | 000334-48-5 | 70   |



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 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP090222.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

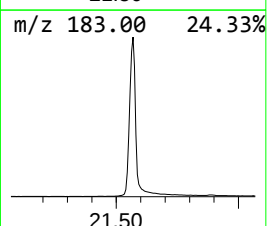
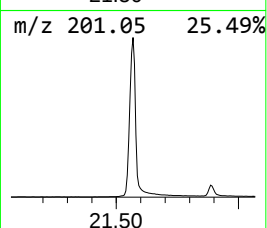
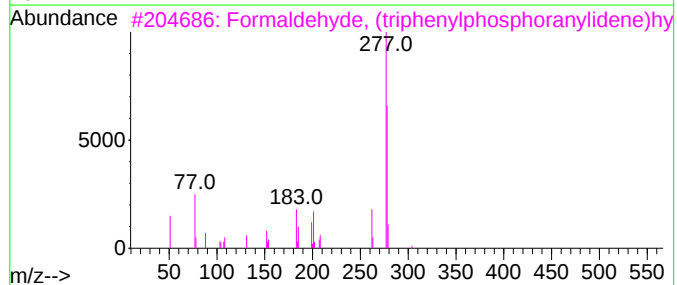
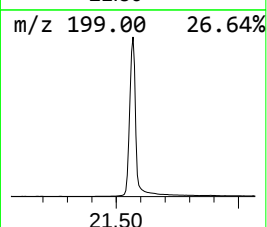
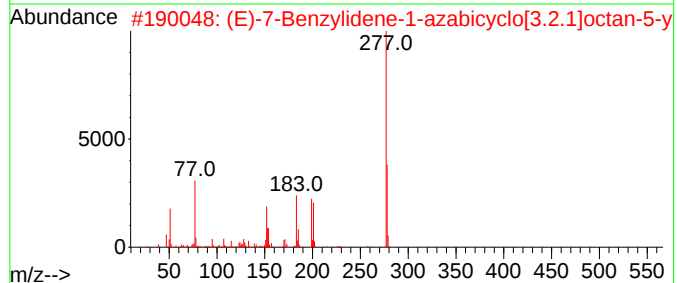
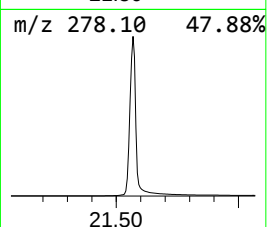
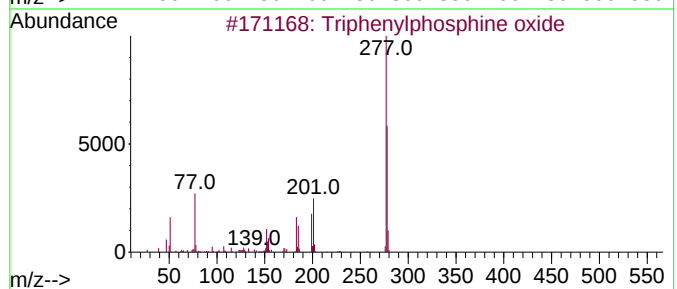
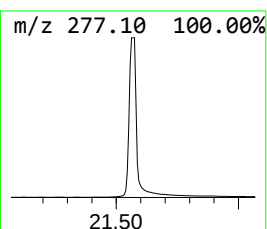
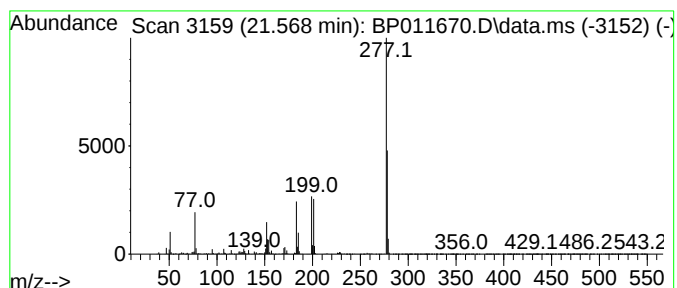
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Peak Number 5 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc   | Area     | Relative to ISTD | R.T.   |
|--------|-----------|----------|------------------|--------|
| 21.569 | 224.20 ng | 59984700 | Chrysene-d12     | 21.433 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 97   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S | 1000483-83-4 | 80   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 64   |
| 4    |    |   | [1,2,4]Triazolo[1,5-a]pyrimidine...  | 278 | C15H14N6   | 1000350-69-0 | 47   |
| 5    |    |   | Quinoline, 2-(2-methyl-5-nitroph...  | 278 | C17H14N2O2 | 311765-54-5  | 37   |



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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... | 3.093  | 139.7   | ng    | 15315100 | 1                     | 7.963  | 2192990 | 20.0 |
| n-Hexadecanoic ... | 18.239 | 3.9     | ng    | 919666   | 4                     | 17.357 | 4676170 | 20.0 |
| Octadecanoic acid  | 19.469 | 2.6     | ng    | 698559   | 5                     | 21.433 | 5351060 | 20.0 |
| Triphenylphosph... | 21.569 | 224.2   | ng    | 59984700 | 5                     | 21.433 | 5351060 | 20.0 |