

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF070622\  
 Data File : BF129142.D  
 Acq On : 06 Jul 2022 14:46  
 Operator : CG\JU  
 Sample : N3562-17  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-16

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-BF062922.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129142.D\data.ms

| peak<br># | R.T.<br>min | first<br>scan | max<br>scan | last<br>scan | PK<br>TY | peak<br>height | corr.<br>area | corr.<br>% max. | % of<br>total |
|-----------|-------------|---------------|-------------|--------------|----------|----------------|---------------|-----------------|---------------|
| 1         | 5.581       | 555           | 560         | 564          | rBV      | 5458685        | 5829745       | 81.32%          | 12.498%       |
| 2         | 6.581       | 724           | 730         | 733          | rBV      | 5086526        | 5751708       | 80.23%          | 12.330%       |
| 3         | 6.957       | 790           | 794         | 797          | rBV      | 1720495        | 1353833       | 18.88%          | 2.902%        |
| 4         | 7.516       | 884           | 889         | 892          | rBV      | 4041542        | 3950119       | 55.10%          | 8.468%        |
| 5         | 8.239       | 1008          | 1012        | 1015         | rBV      | 2110918        | 1755021       | 24.48%          | 3.762%        |
| 6         | 9.316       | 1190          | 1195        | 1198         | rBV      | 7997114        | 7168982       | 100.00%         | 15.369%       |
| 7         | 9.998       | 1307          | 1311        | 1315         | rBV      | 2164865        | 1829760       | 25.52%          | 3.923%        |
| 8         | 10.792      | 1441          | 1446        | 1449         | rBV      | 4251121        | 4092761       | 57.09%          | 8.774%        |
| 9         | 10.892      | 1460          | 1463        | 1469         | rVB      | 58236          | 82653         | 1.15%           | 0.177%        |
| 10        | 11.492      | 1561          | 1565        | 1567         | rBV      | 1968035        | 1649992       | 23.02%          | 3.537%        |
| 11        | 11.516      | 1567          | 1569        | 1573         | rVB      | 145330         | 123269        | 1.72%           | 0.264%        |
| 12        | 11.998      | 1646          | 1651        | 1661         | rBV3     | 441724         | 641075        | 8.94%           | 1.374%        |
| 13        | 12.704      | 1767          | 1771        | 1775         | rBV      | 312020         | 309165        | 4.31%           | 0.663%        |
| 14        | 12.786      | 1780          | 1785        | 1792         | rBV      | 152834         | 197445        | 2.75%           | 0.423%        |
| 15        | 12.939      | 1805          | 1811        | 1817         | rBV      | 926075         | 1191309       | 16.62%          | 2.554%        |
| 16        | 13.080      | 1829          | 1835        | 1838         | rBV      | 6584585        | 5872447       | 81.91%          | 12.589%       |
| 17        | 14.139      | 2011          | 2015        | 2018         | rBV      | 1494859        | 1442306       | 20.12%          | 3.092%        |
| 18        | 14.169      | 2018          | 2020        | 2025         | rVB      | 166328         | 145470        | 2.03%           | 0.312%        |
| 19        | 14.233      | 2027          | 2031        | 2037         | rBV      | 460839         | 469484        | 6.55%           | 1.006%        |
| 20        | 14.286      | 2037          | 2040        | 2047         | rBV      | 72356          | 112774        | 1.57%           | 0.242%        |
| 21        | 14.998      | 2158          | 2161        | 2165         | rVB      | 90042          | 93997         | 1.31%           | 0.202%        |
| 22        | 15.210      | 2194          | 2197        | 2200         | rBV      | 112906         | 158686        | 2.21%           | 0.340%        |
| 23        | 15.268      | 2204          | 2207        | 2214         | rVB      | 116736         | 142562        | 1.99%           | 0.306%        |
| 24        | 15.533      | 2249          | 2252        | 2257         | rVB      | 80306          | 104803        | 1.46%           | 0.225%        |
| 25        | 15.598      | 2259          | 2263        | 2269         | rVV      | 109474         | 150294        | 2.10%           | 0.322%        |
| 26        | 15.668      | 2270          | 2275        | 2285         | rVB      | 1298172        | 1746357       | 24.36%          | 3.744%        |
| 27        | 16.133      | 2351          | 2354        | 2359         | rVB      | 114133         | 165489        | 2.31%           | 0.355%        |
| 28        | 16.674      | 2443          | 2446        | 2453         | rVB      | 67958          | 114694        | 1.60%           | 0.246%        |

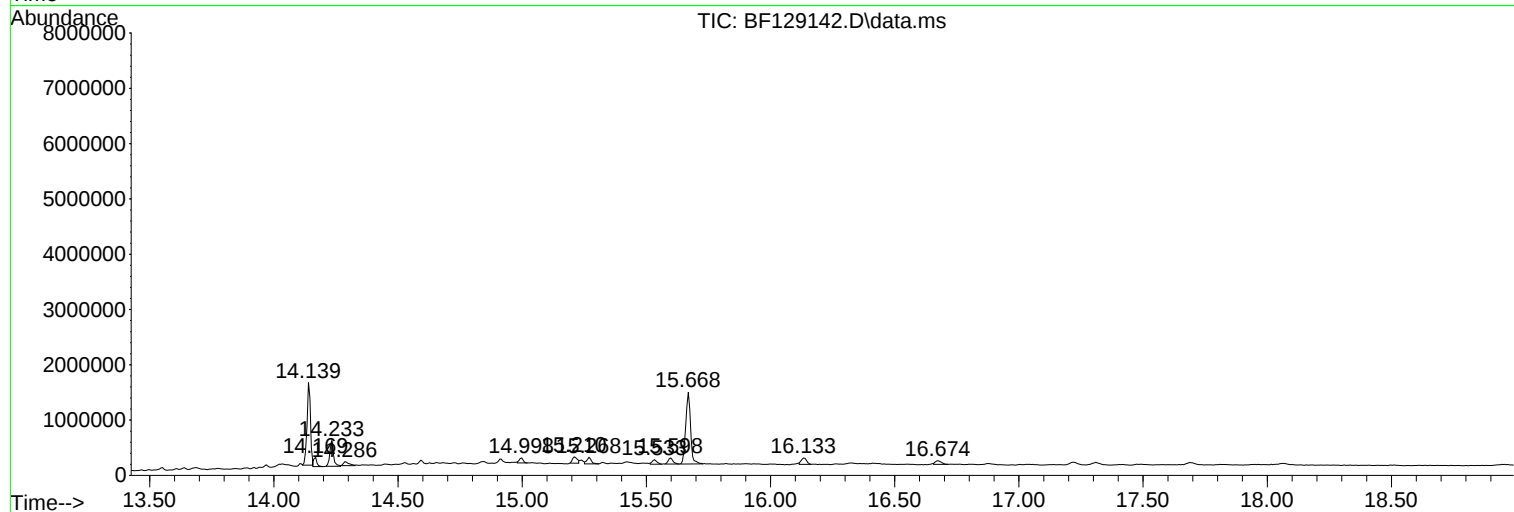
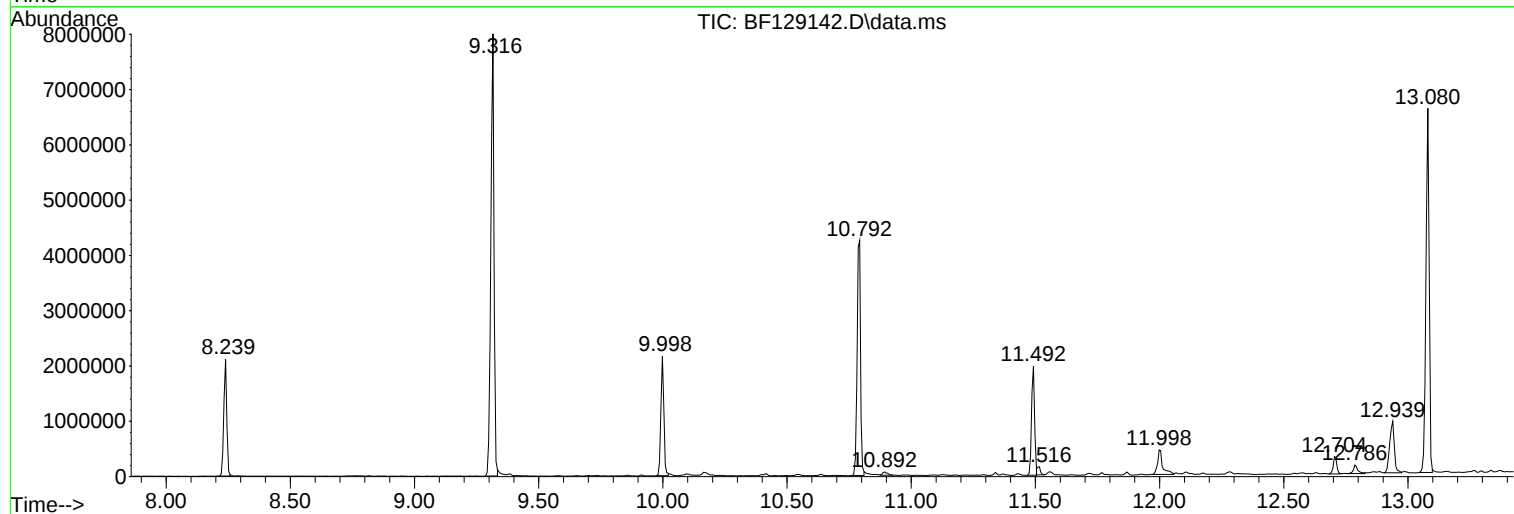
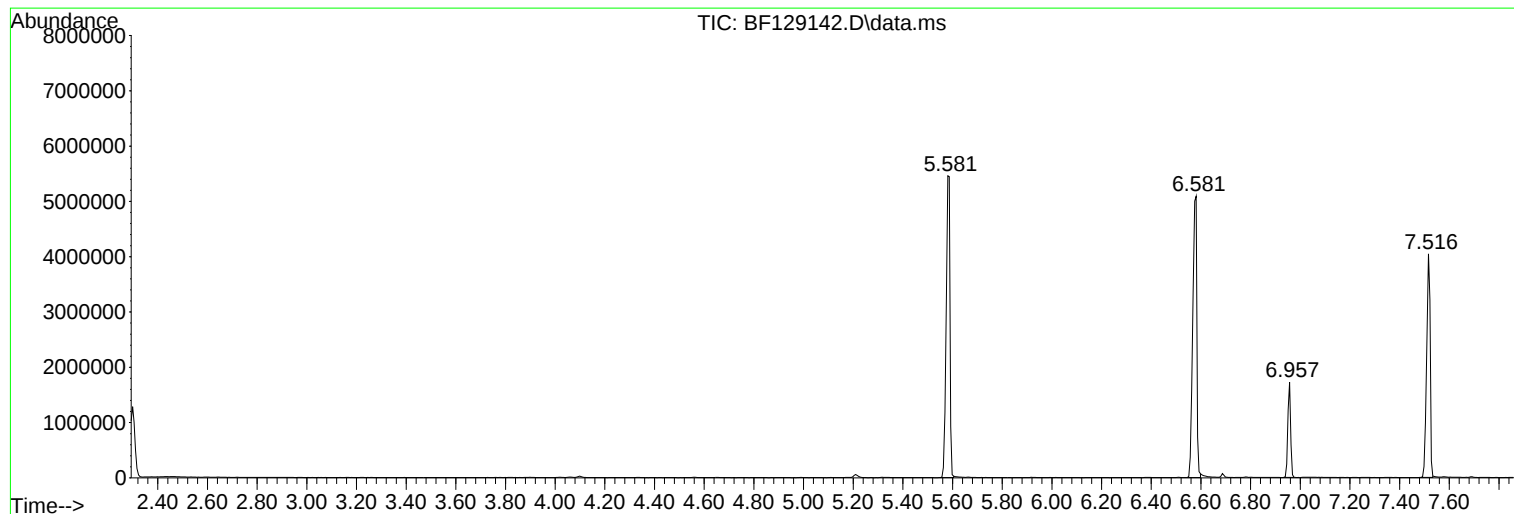
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Instrument :  
BNA\_F  
ClientSampleId :  
SB-16

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.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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BNA\_F  
ClientSampleId :  
SB-16

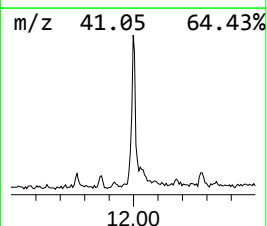
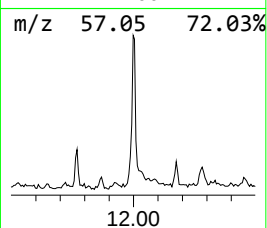
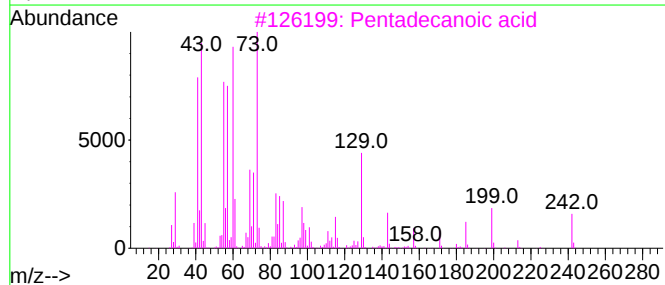
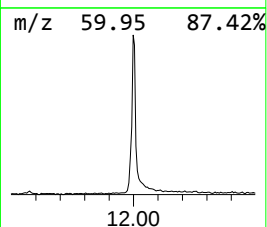
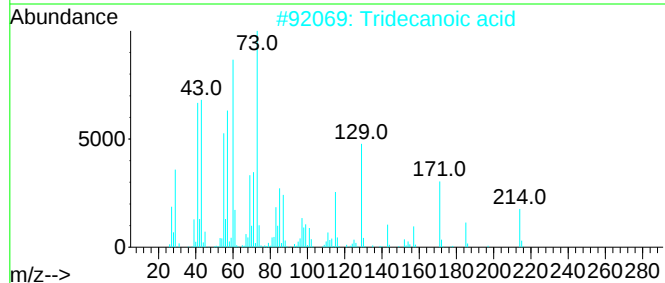
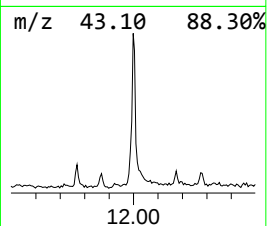
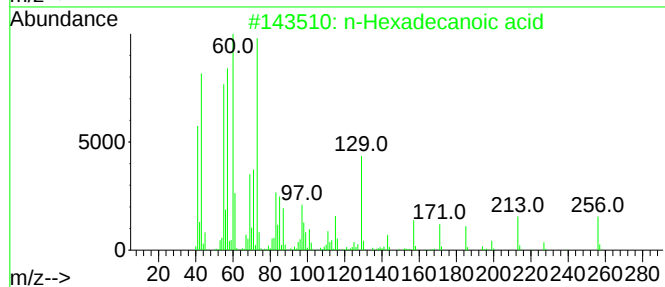
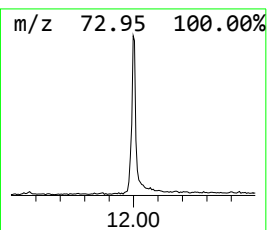
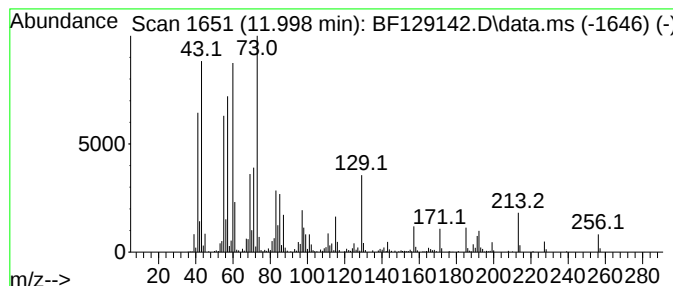
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF062922.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.998 | 7.77 ng | 641075 | Phenanthrene-d10 | 11.492 |

| 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 | 92   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 5    |    |   | Nonanoic acid       | 158 | C9H18O2  | 000112-05-0 | 45   |



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Sample : N3562-17  
Misc :  
ALS Vial : 7 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-16

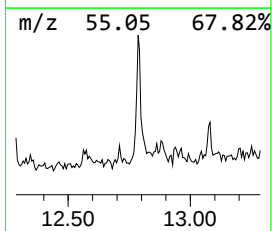
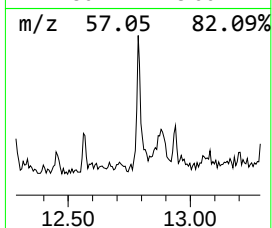
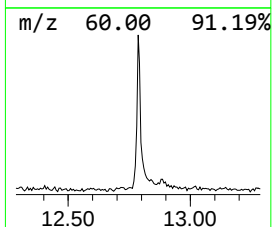
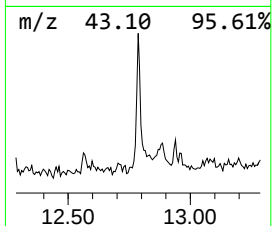
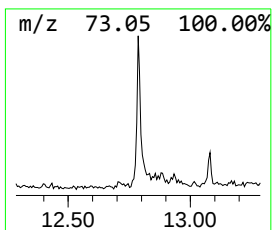
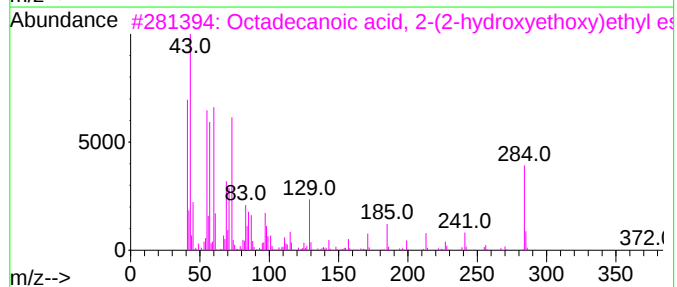
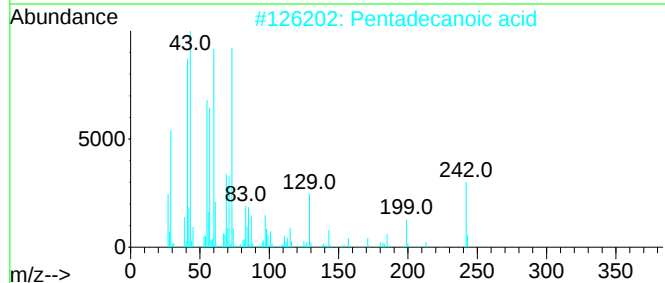
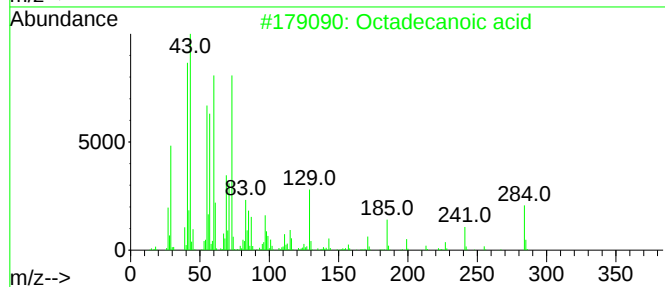
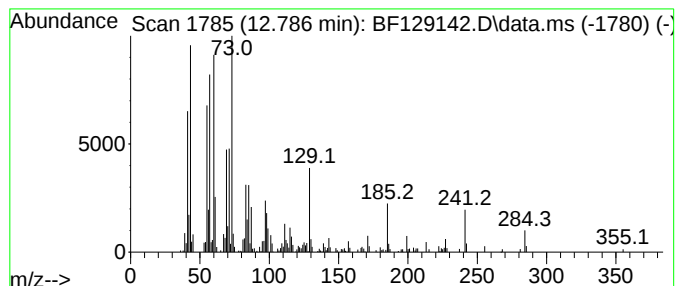
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.786 | 2.39 ng | 197445 | Phenanthrene-d10 | 11.492 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 98   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 93   |
| 3    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 91   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 74   |
| 5    |    |   | Undecanoic acid                     | 186 | C11H22O2 | 000112-37-8 | 60   |



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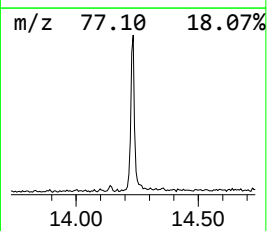
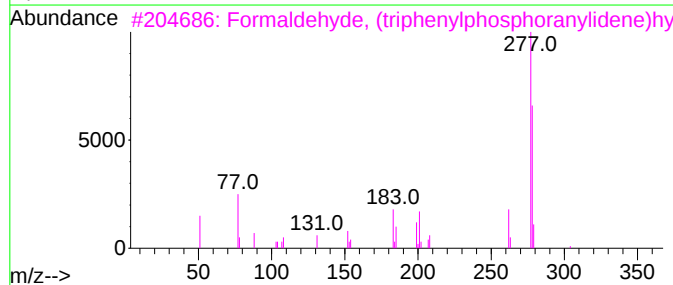
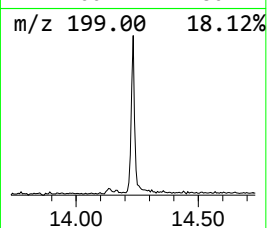
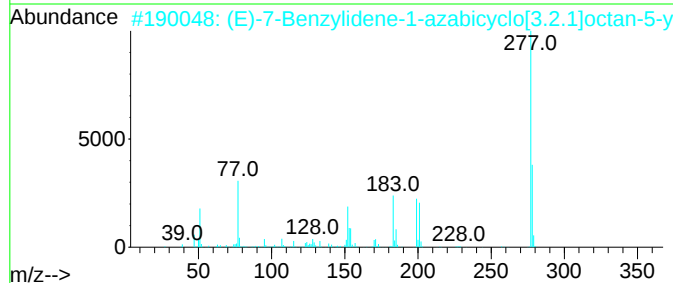
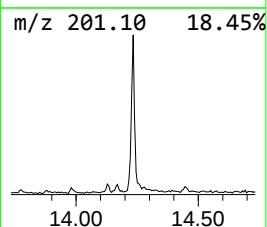
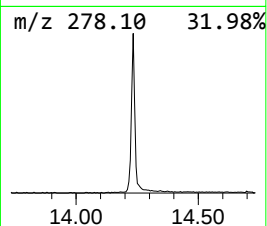
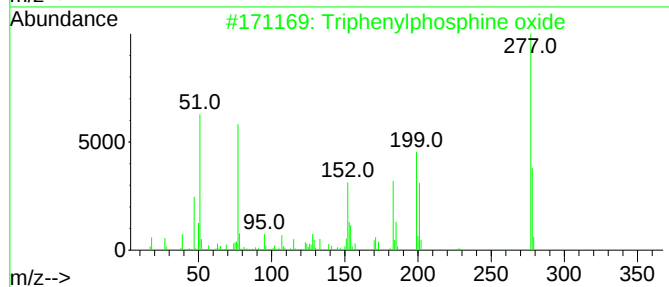
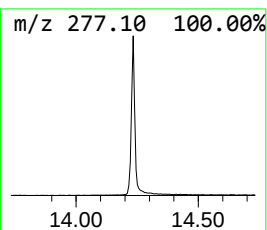
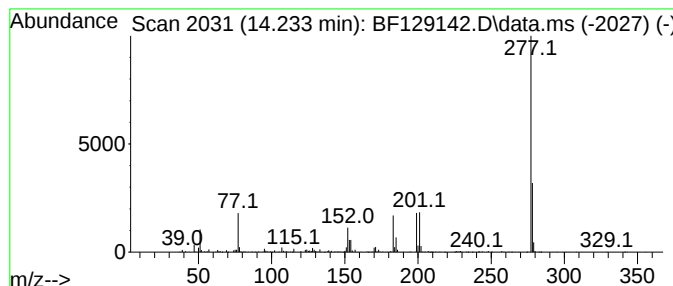
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Triphenylphosphine oxide Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.233 | 6.51 ng | 469484 | Chrysene-d12     | 14.139 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 94   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S  | 1000483-83-4 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 45   |
| 4    |    |   | 1H-Indol-4-ol, 2TMS derivative       | 277 | C14H23NOSi2 | 1000485-28-1 | 33   |
| 5    |    |   | 5-Methyl-8-phenylfuro[3',2':5,6]...  | 277 | C16H11N3O2  | 1000460-07-9 | 28   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| n-Hexadecanoic ... | 11.998 | 7.8     | ng    | 641075   | 4                     | 11.492 | 1649990 | 20.0 |
| Octadecanoic acid  | 12.786 | 2.4     | ng    | 197445   | 4                     | 11.492 | 1649990 | 20.0 |
| Triphenylphosph... | 14.233 | 6.5     | ng    | 469484   | 5                     | 14.139 | 1442310 | 20.0 |