

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP032723\  
 Data File : BP014328.D  
 Acq On : 28 Mar 2023 00:02  
 Operator : CG/JU  
 Sample : 02055-03  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 MW-4

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-BP030623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP014328.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         | 5.105       | 319           | 326         | 340          | rBV      | 376063         | 539357        | 2.80%           | 1.013%        |
| 2         | 5.575       | 399           | 406         | 424          | rBV      | 1081330        | 1707189       | 8.87%           | 3.207%        |
| 3         | 7.187       | 673           | 680         | 707          | rVB      | 560349         | 1098908       | 5.71%           | 2.064%        |
| 4         | 8.022       | 815           | 822         | 832          | rBV      | 505186         | 811458        | 4.21%           | 1.524%        |
| 5         | 9.199       | 1014          | 1022        | 1044         | rBV      | 1693760        | 2953544       | 15.34%          | 5.548%        |
| 6         | 10.846      | 1289          | 1302        | 1316         | rBV      | 579191         | 1036383       | 5.38%           | 1.947%        |
| 7         | 13.292      | 1710          | 1718        | 1741         | rBV      | 4181625        | 6214663       | 32.28%          | 11.673%       |
| 8         | 14.669      | 1945          | 1952        | 1971         | rBV      | 819341         | 1299852       | 6.75%           | 2.442%        |
| 9         | 16.169      | 2200          | 2207        | 2222         | rBV      | 2641354        | 4219777       | 21.92%          | 7.926%        |
| 10        | 17.428      | 2413          | 2421        | 2438         | rBV      | 1002024        | 1581732       | 8.22%           | 2.971%        |
| 11        | 18.292      | 2563          | 2568        | 2580         | rBV      | 179866         | 360684        | 1.87%           | 0.677%        |
| 12        | 19.969      | 2848          | 2853        | 2867         | rBV      | 7061298        | 8312048       | 43.17%          | 15.613%       |
| 13        | 21.510      | 3110          | 3115        | 3122         | rBV      | 1372803        | 1868530       | 9.70%           | 3.510%        |
| 14        | 21.633      | 3130          | 3136        | 3168         | rBV      | 12703095       | 19254022      | 100.00%         | 36.166%       |
| 15        | 24.027      | 3536          | 3543        | 3555         | rVB2     | 916088         | 1980412       | 10.29%          | 3.720%        |

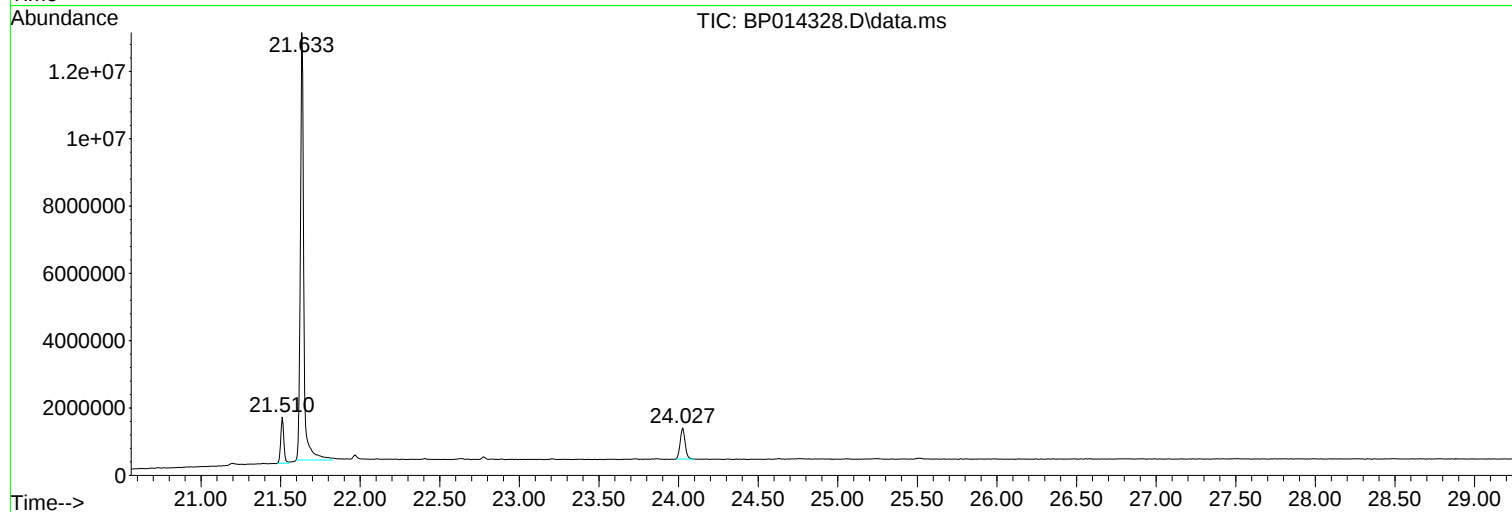
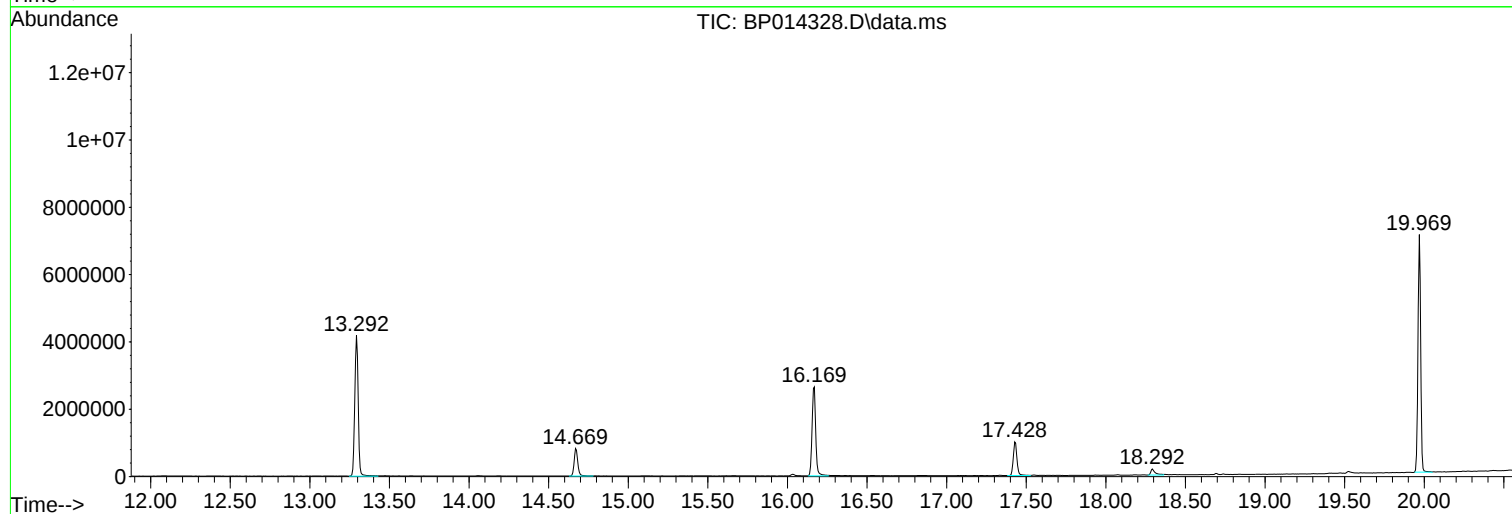
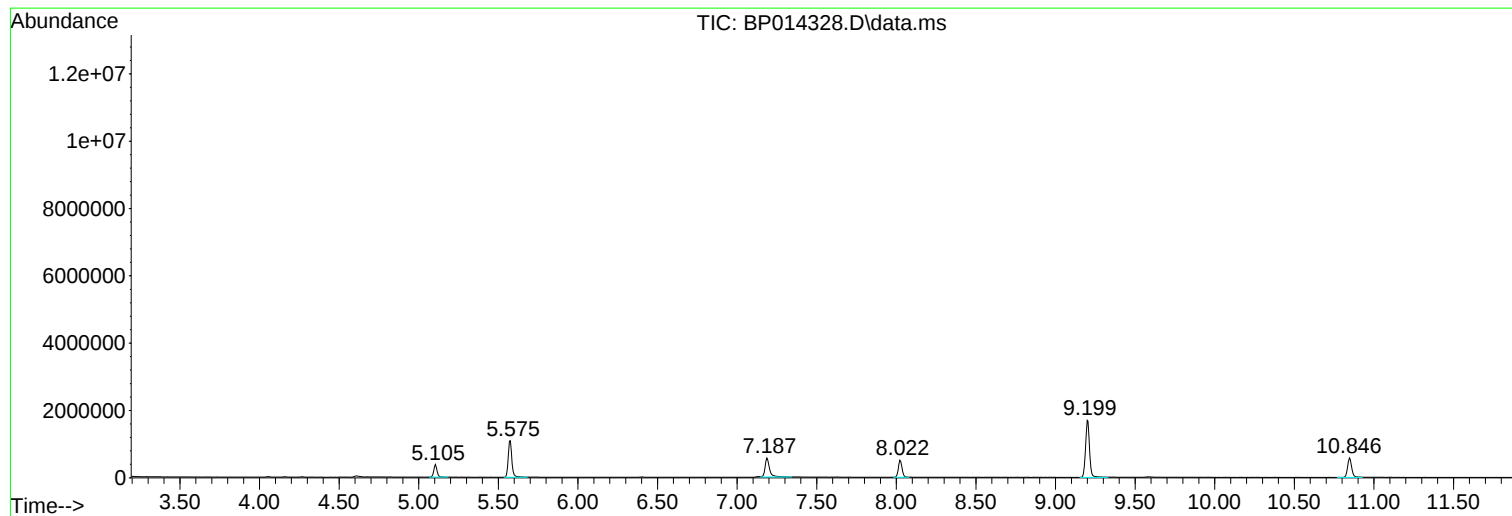
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Instrument :  
BNA\_P  
ClientSampleId :  
MW-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP030623.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

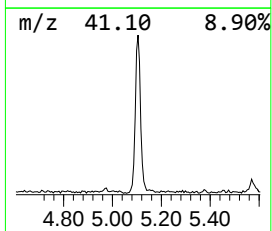
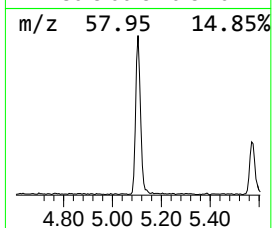
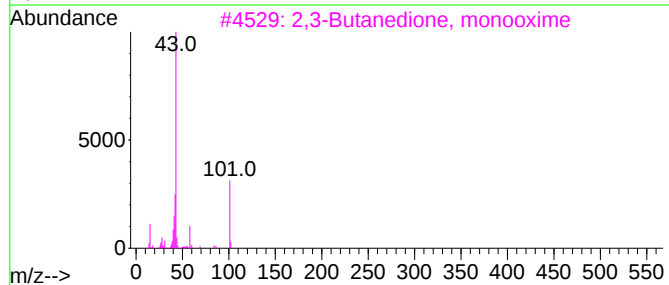
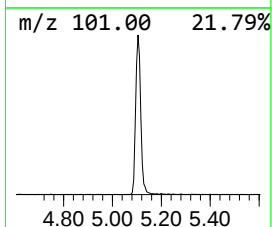
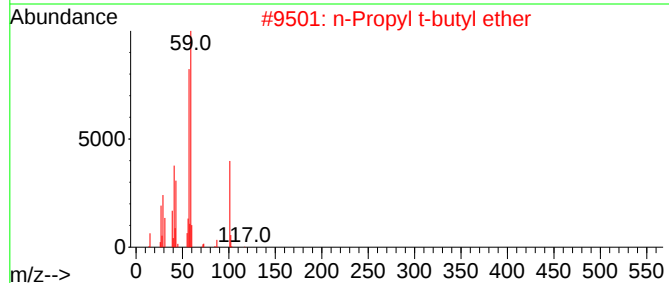
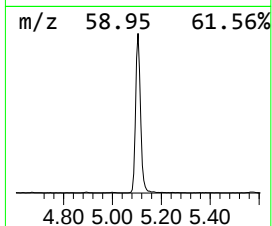
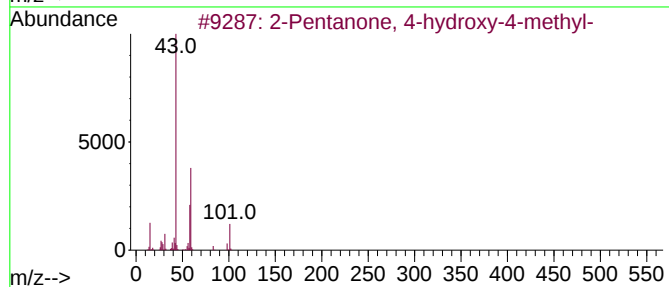
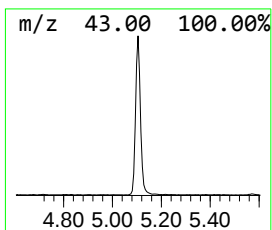
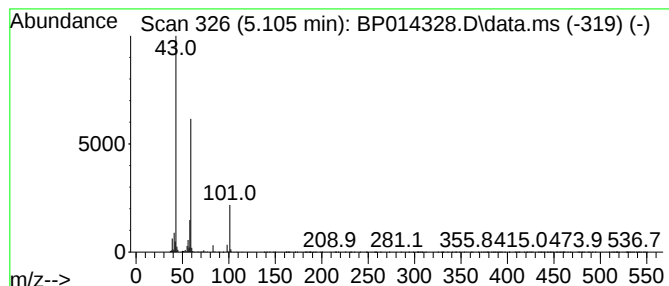
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc  | Area   | Relative to ISTD       | R.T.  |
|-------|----------|--------|------------------------|-------|
| 5.105 | 13.29 ng | 539357 | 1,4-Dichlorobenzene-d4 | 8.022 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2  | 56      |      |      |
| 2    | n-Propyl t-butyl ether              | 116 | C7H16O       | 1000334-81-9 | 33      |      |      |
| 3    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6  | 25      |      |      |
| 4    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9  | 23      |      |      |
| 5    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5  | 10      |      |      |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP030623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

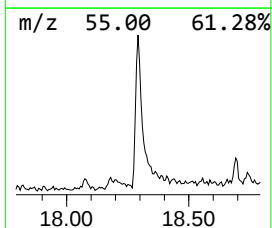
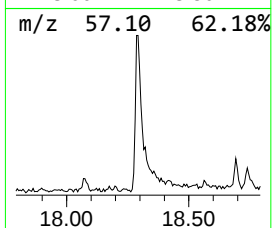
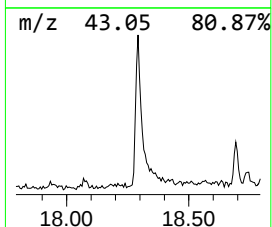
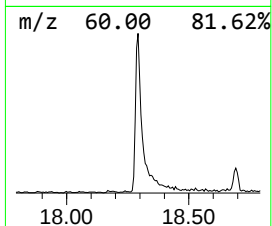
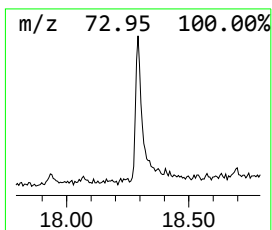
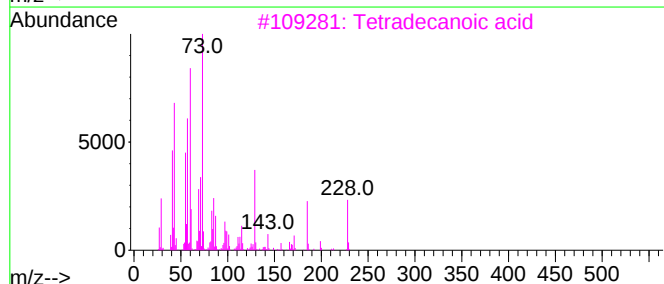
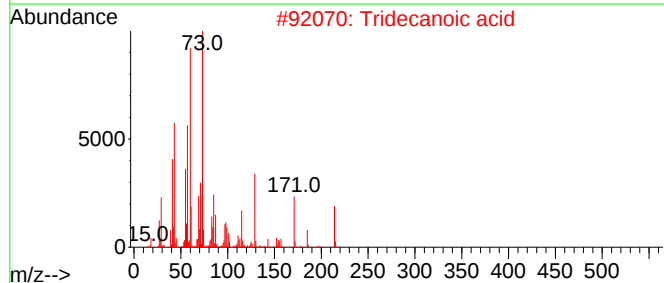
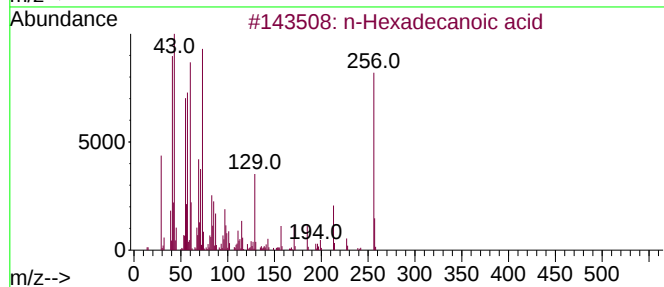
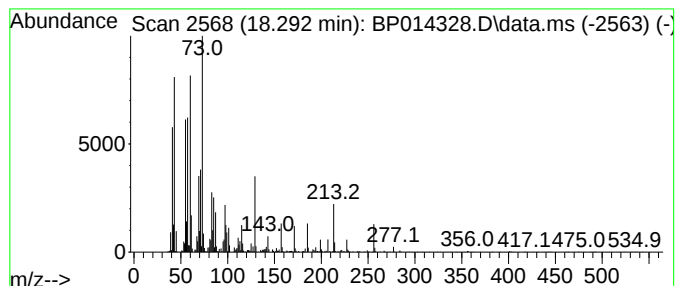
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.292 | 4.56 ng | 360684 | Phenanthrene-d10 | 17.427 |

| 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 | 90   |
| 3    |      | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 86   |
| 4    |      | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 5    |      | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 59   |



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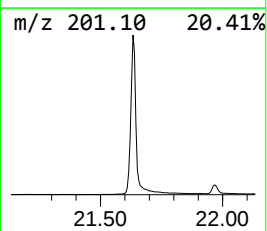
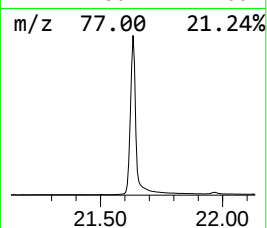
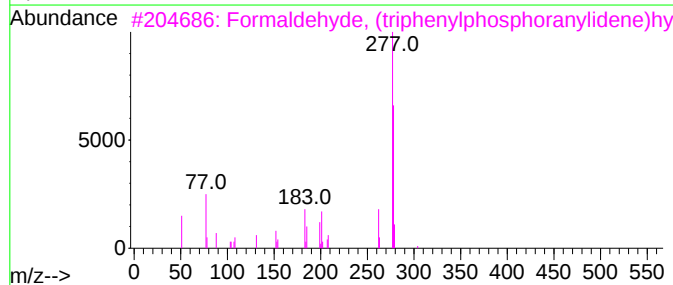
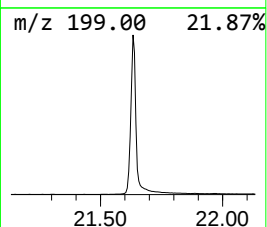
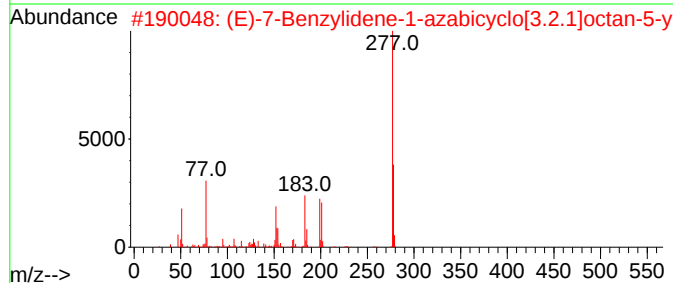
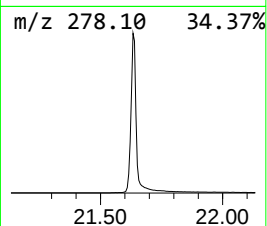
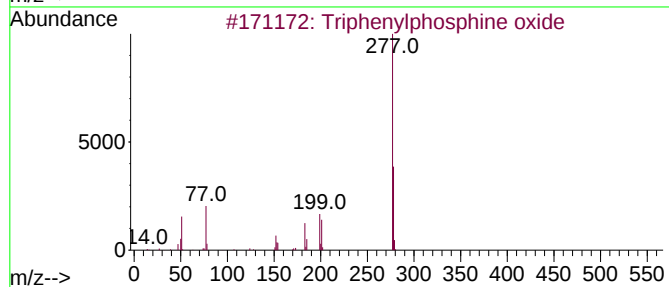
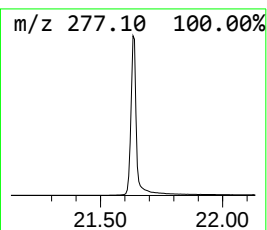
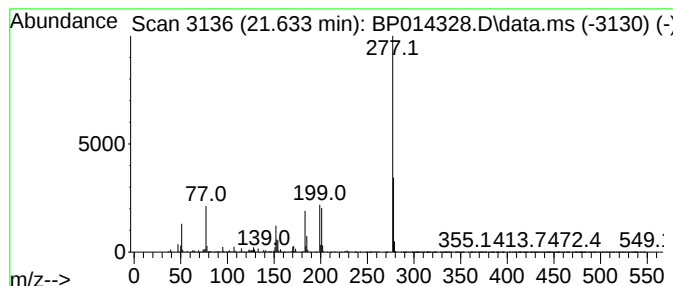
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP030623.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc   | Area     | Relative to ISTD | R.T.   |
|--------|-----------|----------|------------------|--------|
| 21.633 | 206.09 ng | 19254000 | Chrysene-d12     | 21.510 |

| 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 | 91   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 42   |
| 4    |    |   | 1H-Indole-3-acetic acid, 5-[(tri...  | 277 | C14H19N03Si | 072101-35-0  | 25   |
| 5    |    |   | Vanadium, cycloheptatrienyl-(pen...  | 277 | C17H22V     | 1000155-20-5 | 23   |



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BNA\_P  
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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 |
| 2-Pentanone, 4-... | 5.105  | 13.3    | ng    | 539357   | 1                     | 8.022  | 811458  | 20.0 |
| n-Hexadecanoic ... | 18.292 | 4.6     | ng    | 360684   | 4                     | 17.427 | 1581730 | 20.0 |
| Triphenylphosph... | 21.633 | 206.1   | ng    | 19254000 | 5                     | 21.510 | 1868530 | 20.0 |