

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP053122\  
 Data File : BP010639.D  
 Acq On : 31 May 2022 15:33  
 Operator : CG/JU  
 Sample : N3064-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 MW-1

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-BP052822.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP010639.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         | 5.452       | 395           | 402         | 413          | rBV      | 2335431        | 3334534       | 29.61%          | 6.612%        |
| 2         | 7.040       | 664           | 672         | 688          | rBV      | 1530700        | 2546825       | 22.62%          | 5.050%        |
| 3         | 7.863       | 803           | 812         | 822          | rBV      | 646099         | 1042146       | 9.25%           | 2.066%        |
| 4         | 9.028       | 1002          | 1010        | 1026         | rBV      | 2730336        | 4607074       | 40.91%          | 9.135%        |
| 5         | 10.669      | 1277          | 1289        | 1302         | rBV      | 784763         | 1418189       | 12.59%          | 2.812%        |
| 6         | 13.128      | 1696          | 1707        | 1723         | rBV      | 6232966        | 9351199       | 83.04%          | 18.542%       |
| 7         | 14.504      | 1934          | 1941        | 1952         | rBV      | 1131050        | 1816227       | 16.13%          | 3.601%        |
| 8         | 15.998      | 2187          | 2195        | 2213         | rBV      | 4580859        | 6698356       | 59.49%          | 13.282%       |
| 9         | 17.257      | 2402          | 2409        | 2422         | rVB      | 1325798        | 1996482       | 17.73%          | 3.959%        |
| 10        | 18.145      | 2555          | 2560        | 2570         | rBV      | 157405         | 276540        | 2.46%           | 0.548%        |
| 11        | 19.186      | 2734          | 2737        | 2746         | rVB      | 147405         | 174662        | 1.55%           | 0.346%        |
| 12        | 19.380      | 2766          | 2770        | 2781         | rBV      | 241214         | 370297        | 3.29%           | 0.734%        |
| 13        | 19.816      | 2838          | 2844        | 2856         | rBV      | 9538549        | 11260529      | 100.00%         | 22.328%       |
| 14        | 21.051      | 3051          | 3054        | 3061         | rBV      | 150354         | 180528        | 1.60%           | 0.358%        |
| 15        | 21.339      | 3099          | 3103        | 3109         | rBV      | 1196001        | 1557318       | 13.83%          | 3.088%        |
| 16        | 21.457      | 3118          | 3123        | 3132         | rBV      | 1841269        | 2541479       | 22.57%          | 5.039%        |
| 17        | 23.757      | 3508          | 3514        | 3528         | rVB2     | 582110         | 1260615       | 11.19%          | 2.500%        |

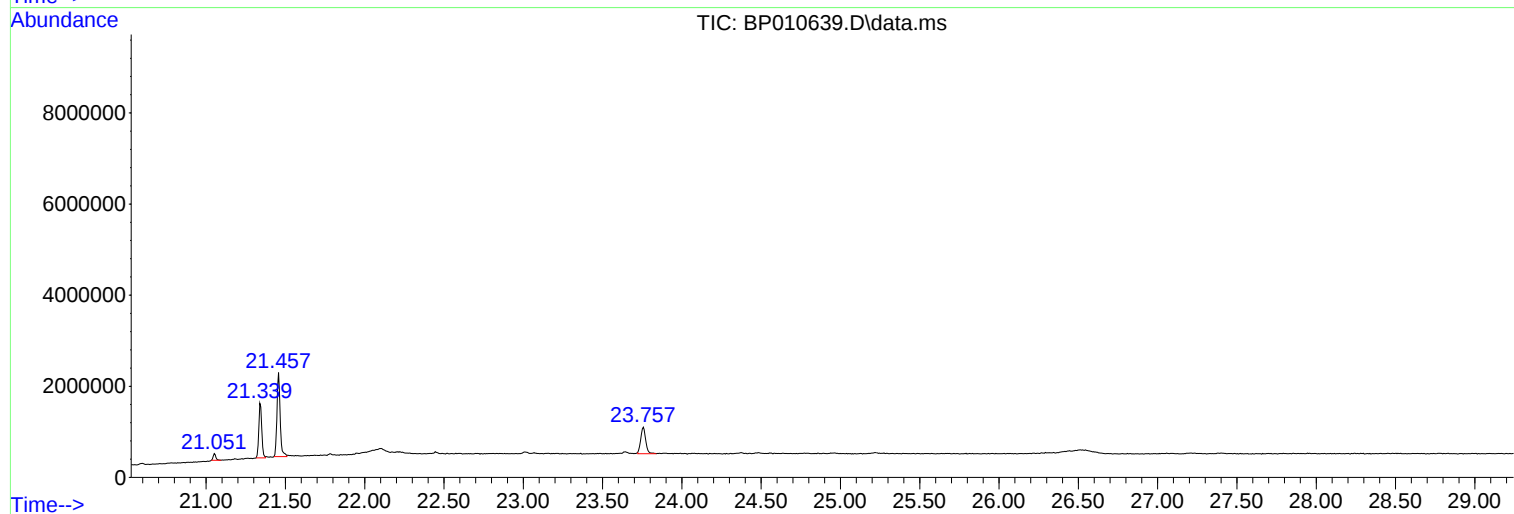
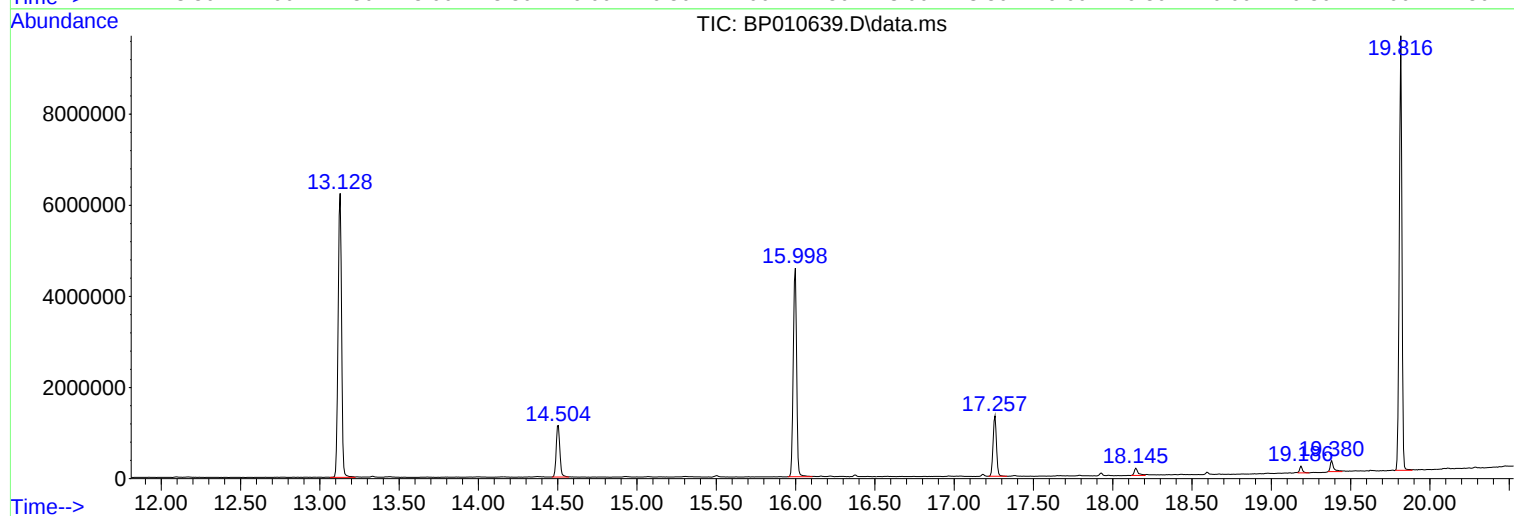
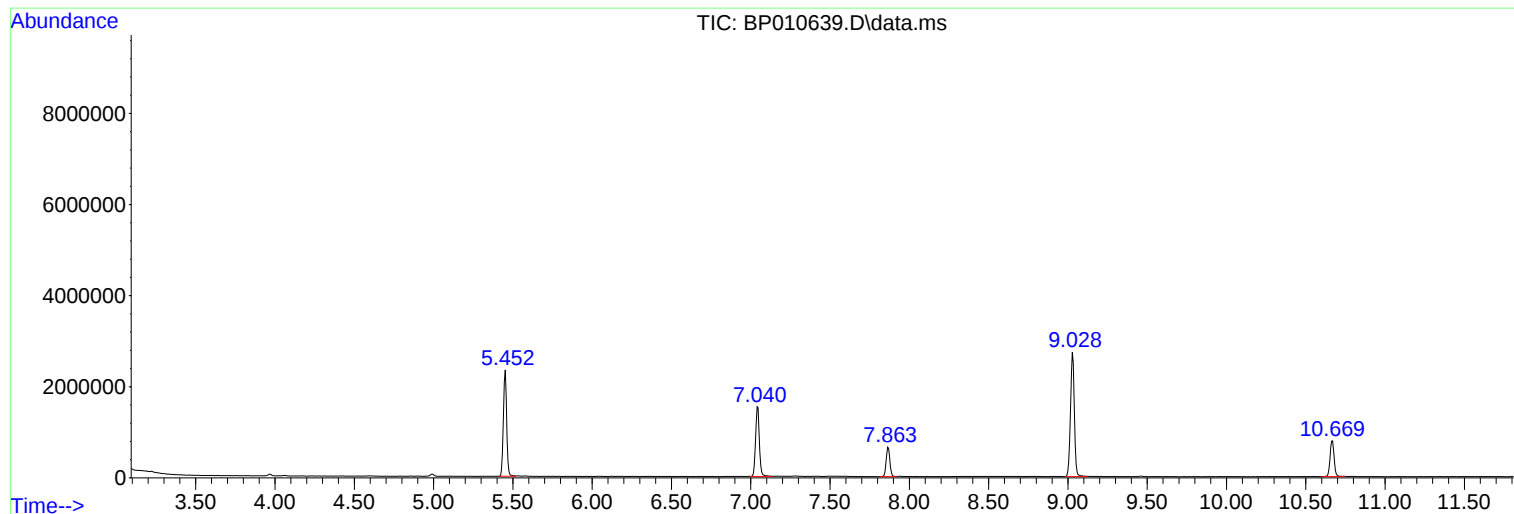
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BNA\_P  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP052822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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MW-1

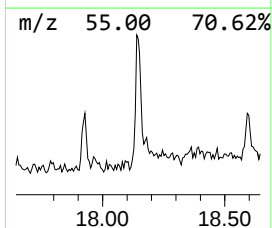
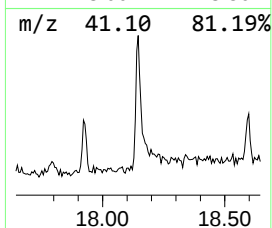
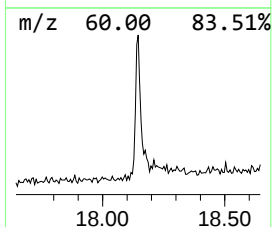
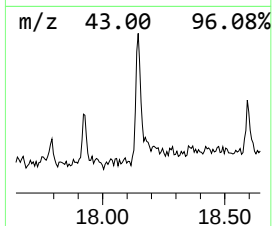
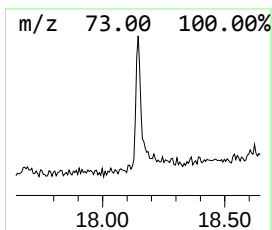
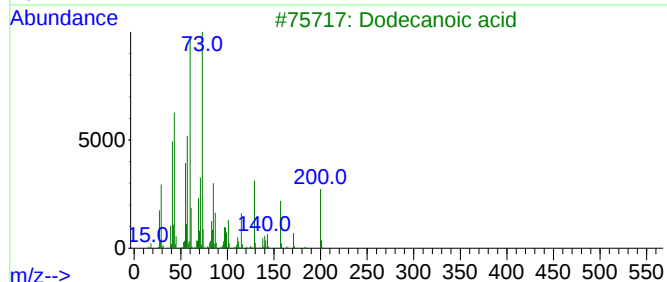
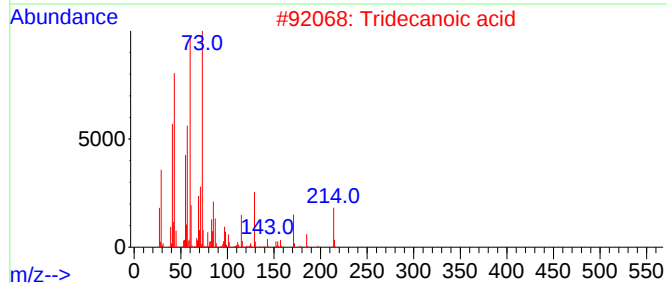
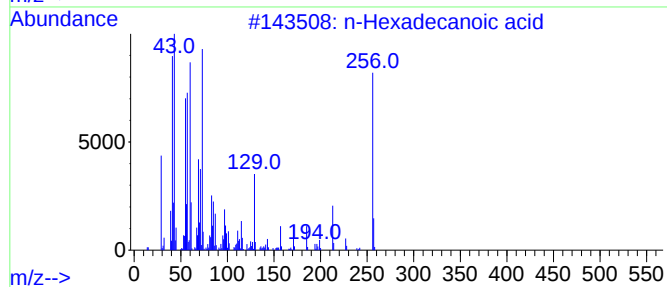
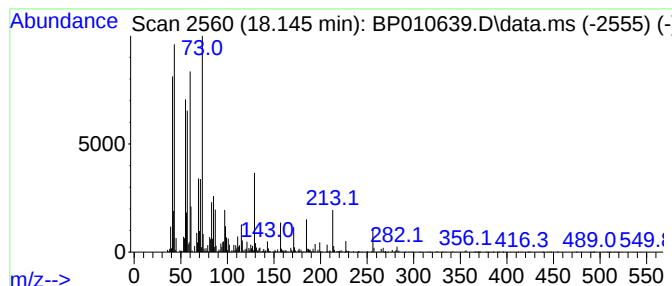
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP052822.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.145 | 2.77 ng | 276540 | Phenanthrene-d10 | 17.257 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 94   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 81   |
| 3    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 68   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 64   |



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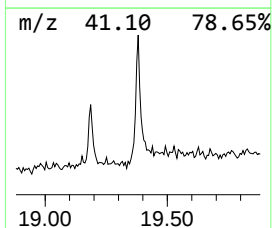
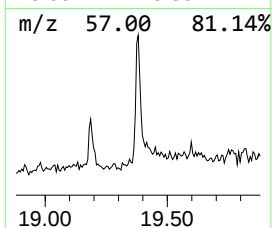
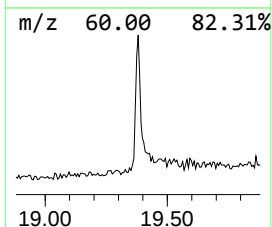
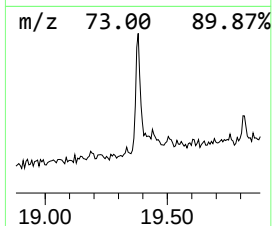
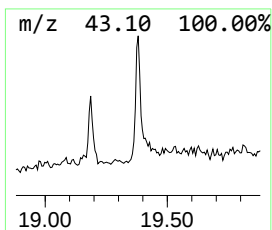
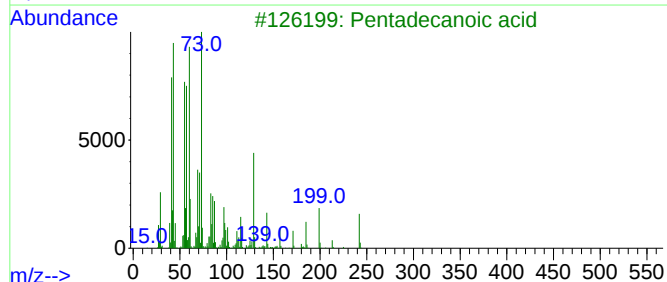
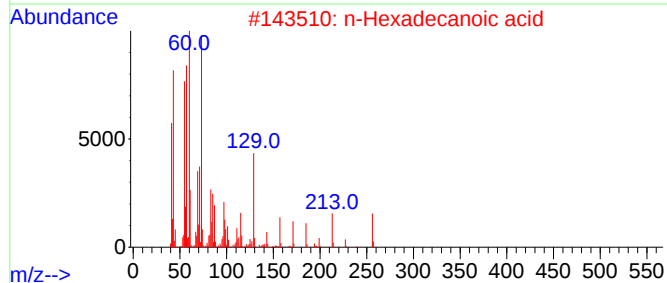
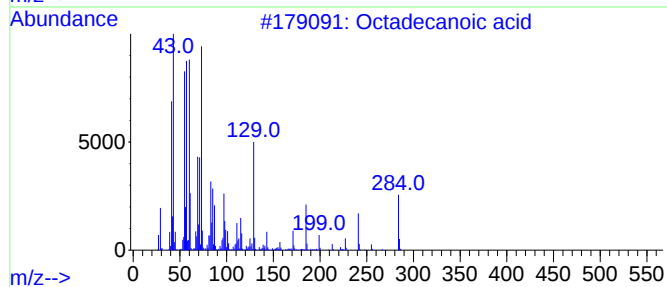
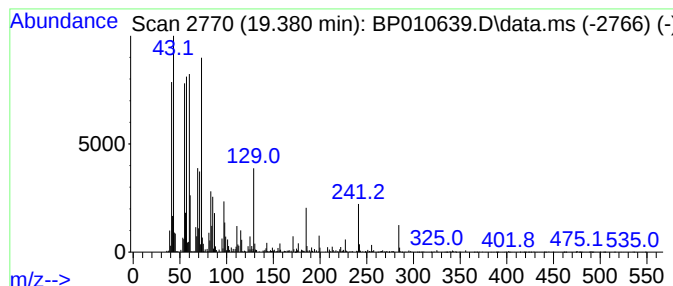
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP052822.M  
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TIC Library : C:\Database\NIST20.L  
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Peak Number 2 Octadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.380 | 4.76 ng | 370297 | Chrysene-d12     | 21.339 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | n-Hexadecanoic acid                 | 256 | C16H32O2 | 000057-10-3 | 72   |
| 3    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 72   |
| 4    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 68   |
| 5    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 64   |



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Misc :  
ALS Vial : 6 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
MW-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP052822.M  
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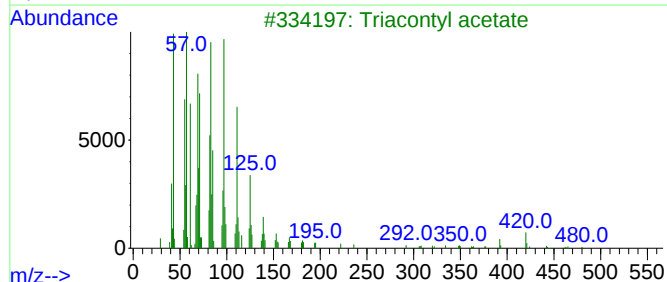
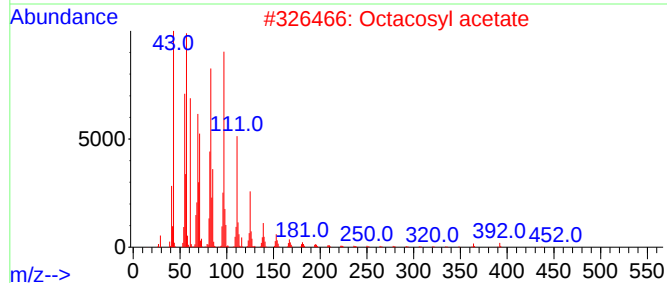
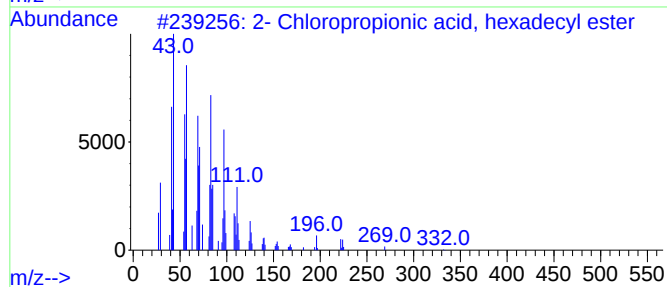
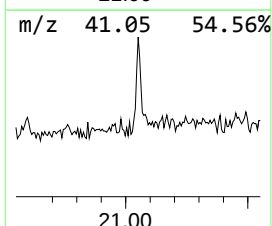
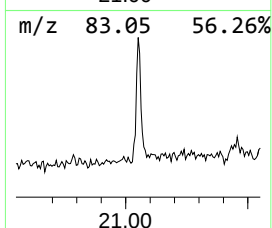
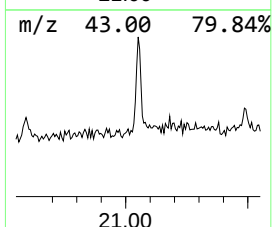
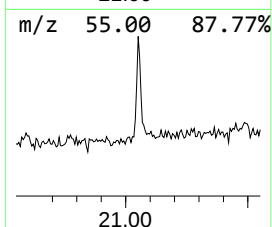
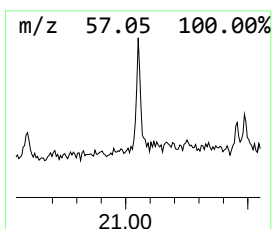
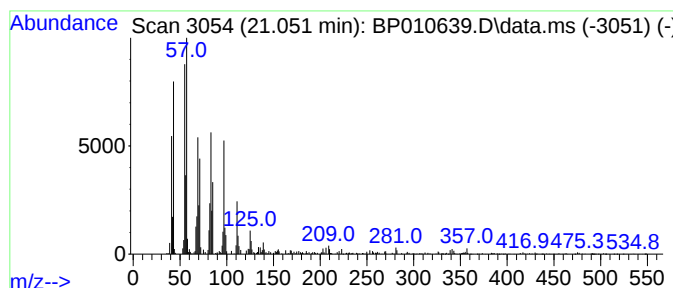
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 2- Chloropropionic acid, he... Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.051 | 2.32 ng | 180528 | Chrysene-d12     | 21.339 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | 2- Chloropropionic acid, hexadec... | 332 | C19H37ClO2 | 086711-81-1  | 96   |
| 2    |    |   | Octacosyl acetate                   | 452 | C30H60O2   | 018206-97-8  | 93   |
| 3    |    |   | Triacontyl acetate                  | 480 | C32H64O2   | 041755-58-2  | 93   |
| 4    |    |   | Nonadecyl pentafluoropropionate     | 430 | C22H39F5O2 | 1000351-88-8 | 91   |
| 5    |    |   | Eicosyl trifluoroacetate            | 394 | C22H41F3O2 | 1000351-75-2 | 91   |



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ALS Vial : 6 Sample Multiplier: 1

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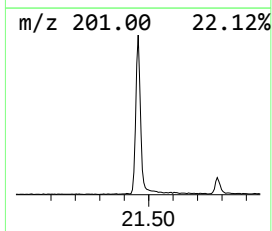
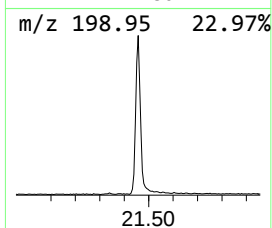
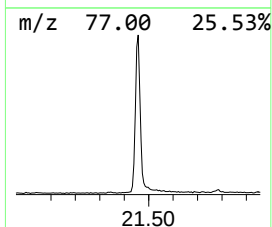
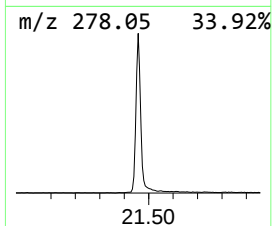
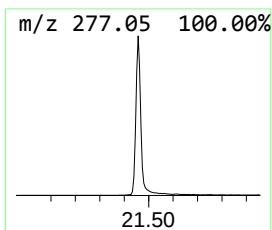
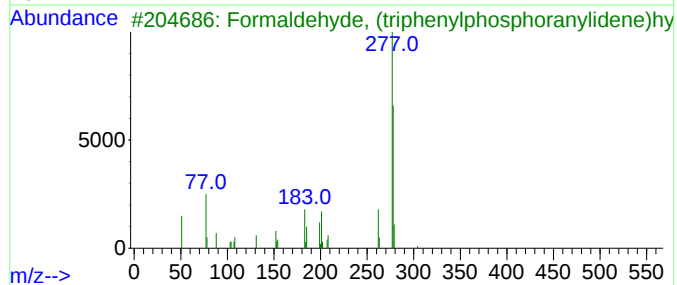
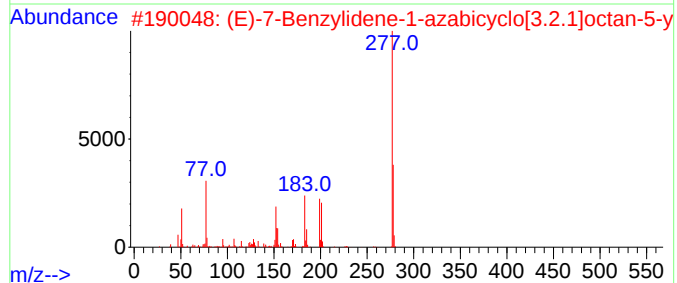
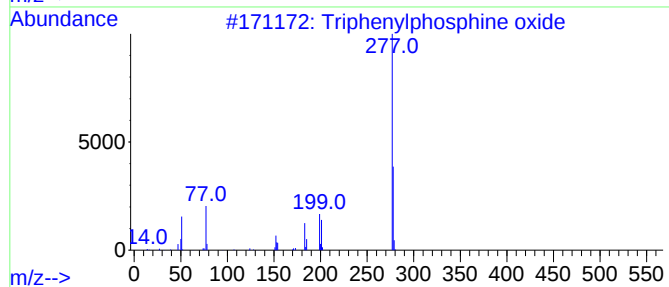
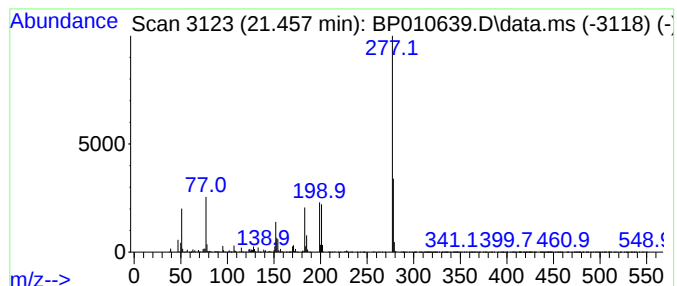
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TIC Library : C:\Database\NIST20.L  
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc  | Area    | Relative to ISTD | R.T.   |
|--------|----------|---------|------------------|--------|
| 21.457 | 32.64 ng | 2541480 | Chrysene-d12     | 21.339 |

| 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 | C15H19NO3S  | 1000483-83-4 | 81   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...] | 304 | C19H17N2P   | 015990-54-2  | 50   |
| 4    |    |   | 3-(3,4-Dichlorophenyl)-2-thioxo-...  | 277 | C9H5Cl2NOS2 | 017046-34-3  | 25   |
| 5    |    |   | Carbazol-1-one, 1,2,3,4-tetrahyd...  | 277 | C18H15NO2   | 299962-12-2  | 23   |



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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 |
| n-Hexadecanoic ... | 18.145 | 2.8     | ng    | 276540   | 4                     | 17.257 | 1996480 | 20.0 |
| Octadecanoic acid  | 19.380 | 4.8     | ng    | 370297   | 5                     | 21.339 | 1557320 | 20.0 |
| 2- Chloropropio... | 21.051 | 2.3     | ng    | 180528   | 5                     | 21.339 | 1557320 | 20.0 |
| Triphenylphosph... | 21.457 | 32.6    | ng    | 2541480  | 5                     | 21.339 | 1557320 | 20.0 |