

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF090122\  
 Data File : BF130085.D  
 Acq On : 01 Sep 2022 19:15  
 Operator : CG\JU  
 Sample : N4385-02  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 265751-2

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-BF083122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130085.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         | 4.893       | 439           | 443         | 451          | rVB      | 182326         | 204702        | 3.10%           | 0.584%        |
| 2         | 5.304       | 508           | 513         | 516          | rBV      | 2504340        | 2492889       | 37.73%          | 7.115%        |
| 3         | 6.322       | 682           | 686         | 689          | rBV      | 1777687        | 1465466       | 22.18%          | 4.183%        |
| 4         | 6.704       | 747           | 751         | 754          | rBV      | 1467591        | 1299599       | 19.67%          | 3.709%        |
| 5         | 7.269       | 841           | 847         | 850          | rBV      | 3781869        | 3658317       | 55.37%          | 10.441%       |
| 6         | 7.981       | 964           | 968         | 972          | rBV      | 1976714        | 1743948       | 26.39%          | 4.977%        |
| 7         | 8.369       | 1031          | 1034        | 1048         | rBV      | 188638         | 206355        | 3.12%           | 0.589%        |
| 8         | 9.063       | 1146          | 1152        | 1155         | rBV      | 6777480        | 6607398       | 100.00%         | 18.858%       |
| 9         | 9.734       | 1261          | 1266        | 1269         | rBV      | 2481877        | 1993668       | 30.17%          | 5.690%        |
| 10        | 10.522      | 1395          | 1400        | 1403         | rBV      | 4328715        | 4000496       | 60.55%          | 11.418%       |
| 11        | 11.216      | 1514          | 1518        | 1521         | rBV      | 2172479        | 1912794       | 28.95%          | 5.459%        |
| 12        | 11.616      | 1583          | 1586        | 1591         | rVB      | 121069         | 107128        | 1.62%           | 0.306%        |
| 13        | 11.751      | 1605          | 1609        | 1612         | rBV      | 100458         | 103978        | 1.57%           | 0.297%        |
| 14        | 12.322      | 1699          | 1706        | 1709         | rBV      | 343841         | 294324        | 4.45%           | 0.840%        |
| 15        | 12.410      | 1718          | 1721        | 1725         | rBV      | 89147          | 71975         | 1.09%           | 0.205%        |
| 16        | 12.804      | 1783          | 1788        | 1791         | rBV      | 6105864        | 5993672       | 90.71%          | 17.106%       |
| 17        | 13.845      | 1961          | 1965        | 1968         | rVB      | 1543947        | 1426373       | 21.59%          | 4.071%        |
| 18        | 13.945      | 1978          | 1982        | 1988         | rVB      | 177133         | 184430        | 2.79%           | 0.526%        |
| 19        | 14.692      | 2106          | 2109        | 2112         | rBV      | 84604          | 78151         | 1.18%           | 0.223%        |
| 20        | 15.245      | 2198          | 2203        | 2208         | rBV      | 1038384        | 1192353       | 18.05%          | 3.403%        |

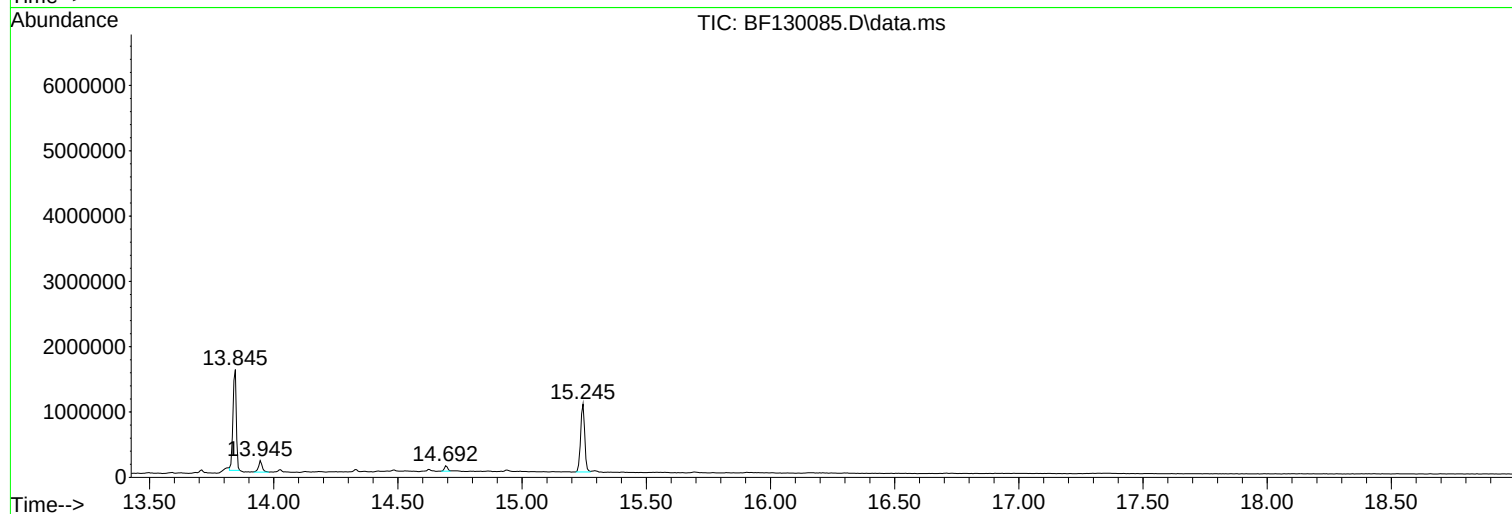
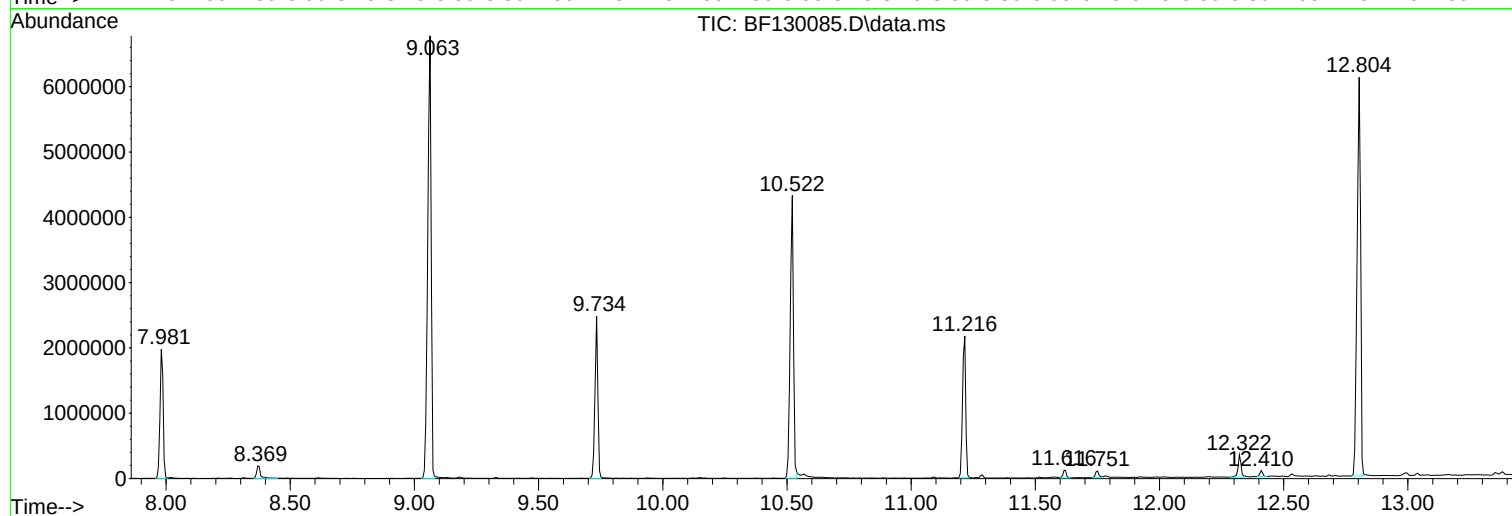
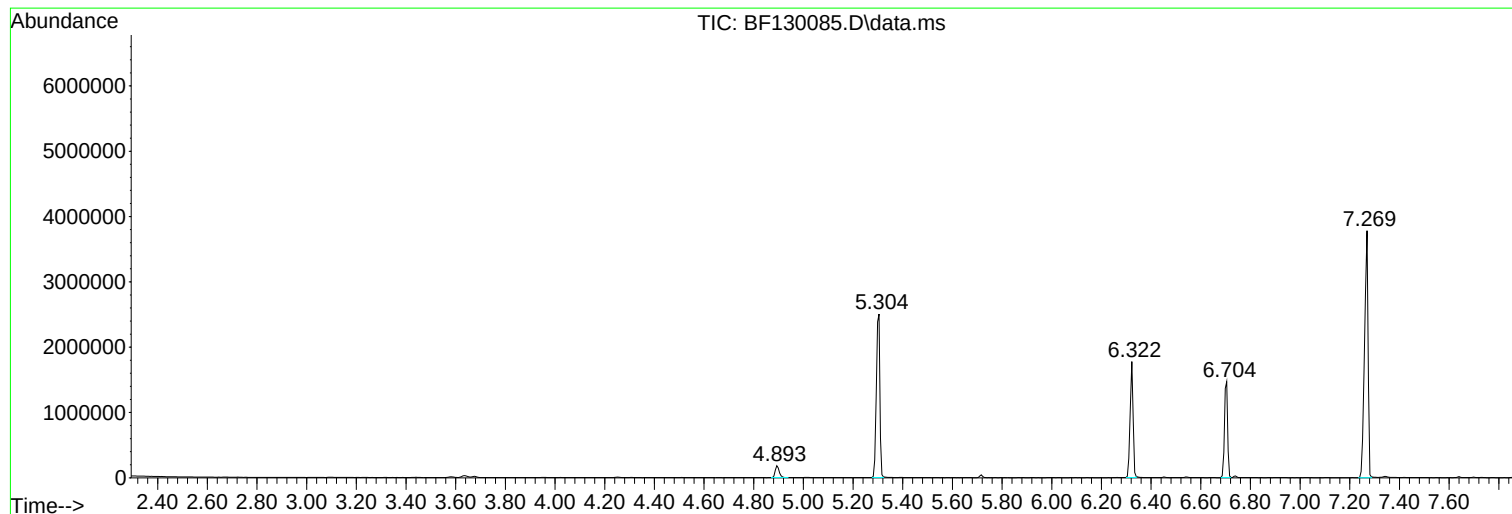
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Misc :  
ALS Vial : 7 Sample Multiplier: 1

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BNA\_F  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083122.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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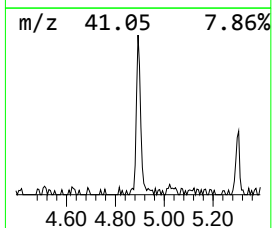
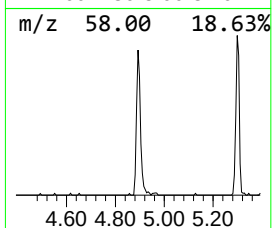
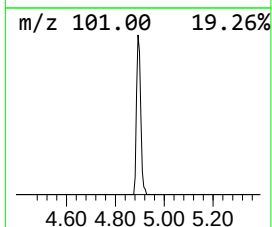
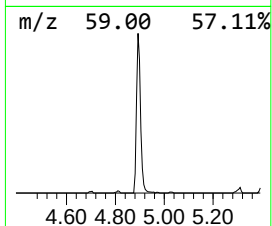
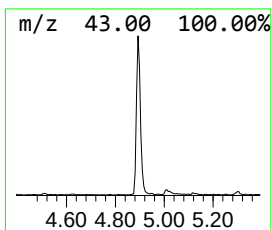
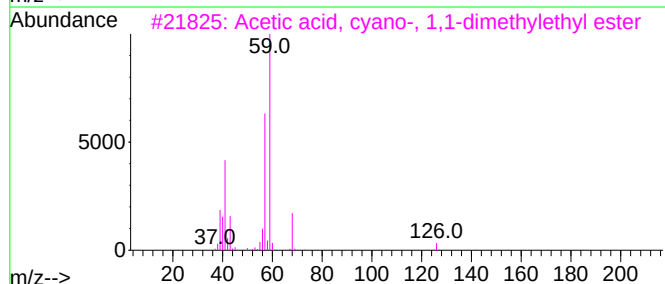
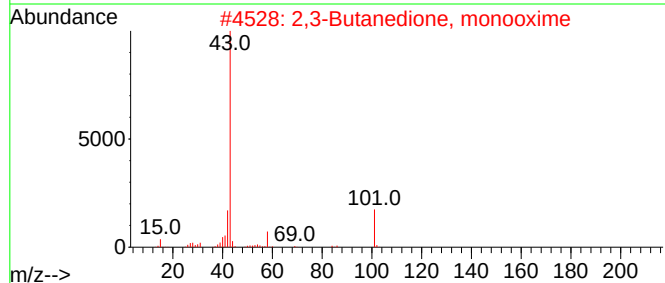
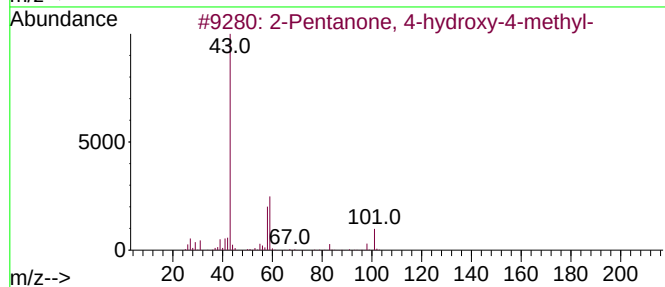
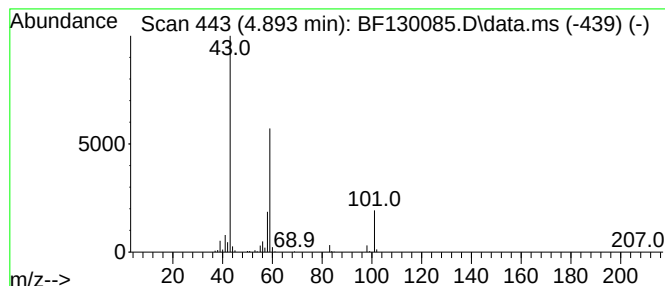
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area   | Relative to ISTD       | R.T.  |
|-------|---------|--------|------------------------|-------|
| 4.893 | 3.15 ng | 204702 | 1,4-Dichlorobenzene-d4 | 6.704 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2      | 000057-71-6 | 25      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | 1-Propen-2-ol, acetate              | 100 | C5H8O2       | 000108-22-5 | 10      |      |      |
| 5    | Morpholine, 4-methyl-               | 101 | C5H11NO      | 000109-02-4 | 9       |      |      |



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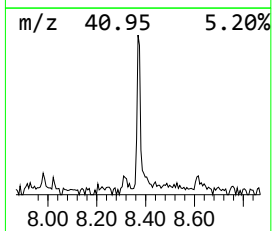
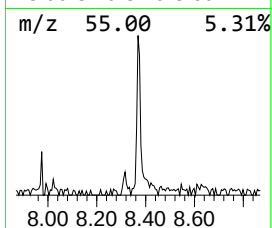
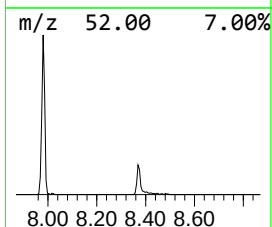
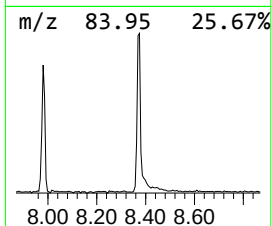
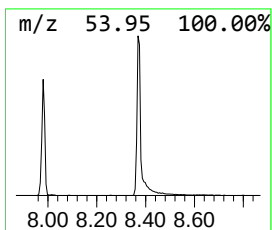
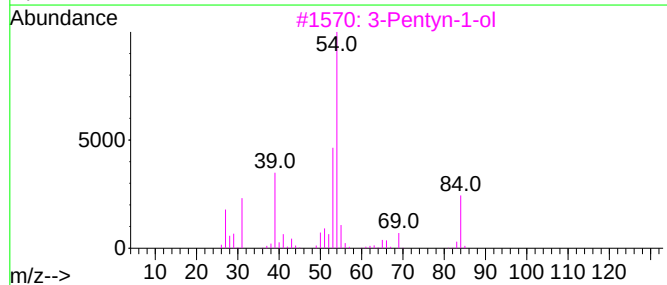
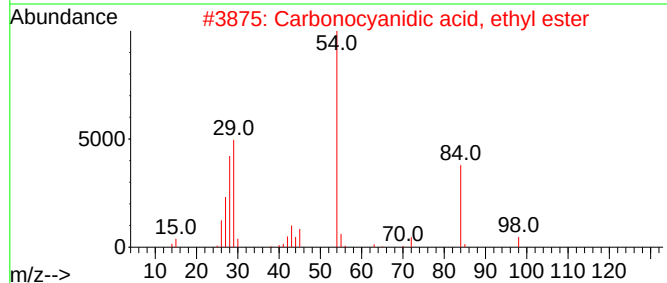
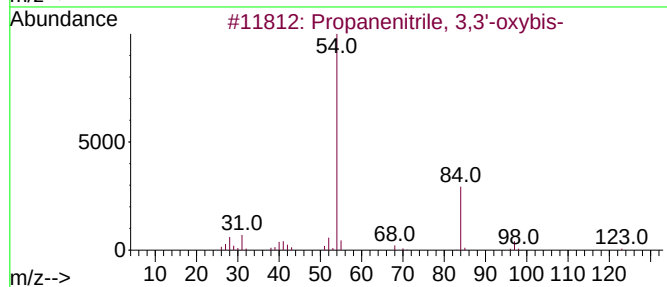
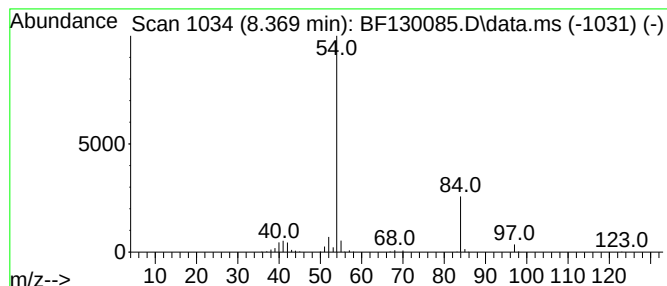
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF083122.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Propanenitrile, 3,3'-oxybis- Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.369 | 2.37 ng | 206355 | Naphthalene-d8   | 7.981 |

| Hit# | of | 5 | Tentative ID                      | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------------|-----|---------|-------------|------|
| 1    |    |   | Propanenitrile, 3,3'-oxybis-      | 124 | C6H8N2O | 001656-48-0 | 83   |
| 2    |    |   | Carbonocyanidic acid, ethyl ester | 99  | C4H5NO2 | 000623-49-4 | 64   |
| 3    |    |   | 3-Pentyn-1-ol                     | 84  | C5H8O   | 010229-10-4 | 64   |
| 4    |    |   | 2-Butyne                          | 54  | C4H6    | 000503-17-3 | 9    |
| 5    |    |   | 1-Butyne                          | 54  | C4H6    | 000107-00-6 | 7    |



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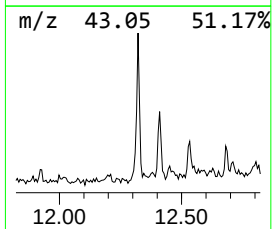
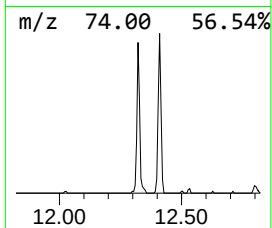
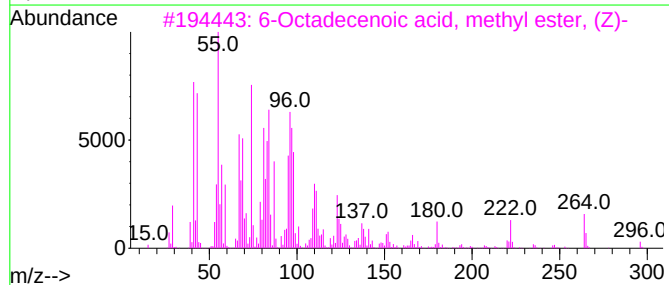
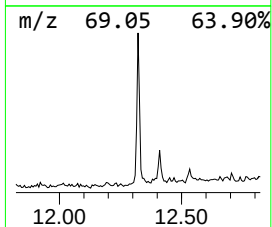
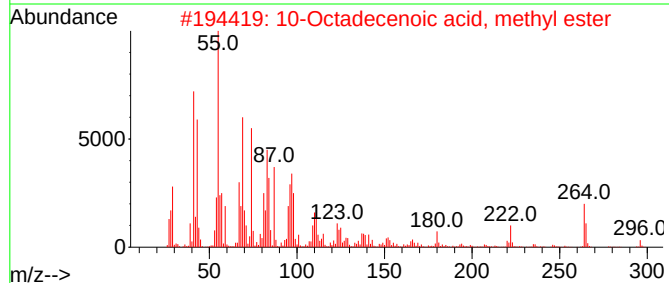
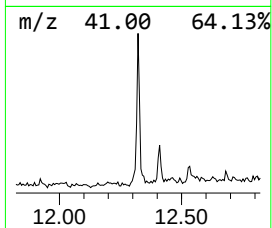
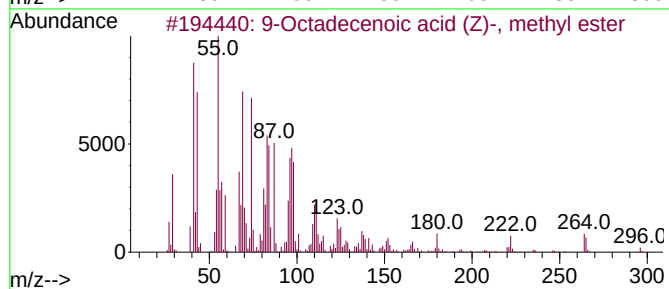
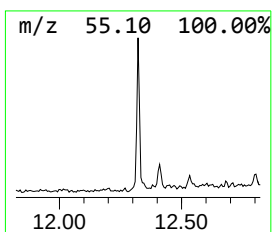
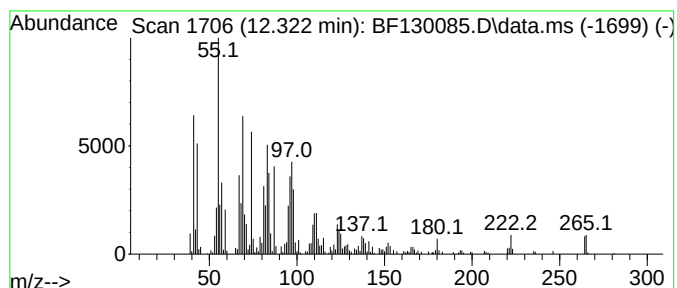
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Peak Number 3 9-Octadecenoic acid (Z)-, m... Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|--------------|------|
| 12.322    | 3.08 ng                             | 294324 | Phenanthrene-d10 | 11.216       |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#         | Qual |
| 1         | 9-Octadecenoic acid (Z)-, methyl... | 296    | C19H36O2         | 000112-62-9  | 95   |
| 2         | 10-Octadecenoic acid, methyl ester  | 296    | C19H36O2         | 013481-95-3  | 94   |
| 3         | 6-Octadecenoic acid, methyl este... | 296    | C19H36O2         | 002777-58-4  | 93   |
| 4         | trans-13-Octadecenoic acid, meth... | 296    | C19H36O2         | 1000333-61-3 | 91   |
| 5         | 14-Octadecenoic acid, methyl ester  | 296    | C19H36O2         | 056554-48-4  | 91   |



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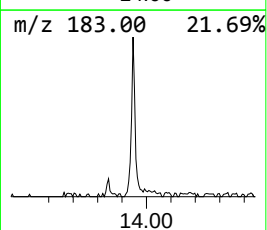
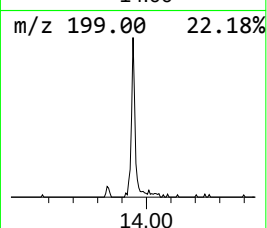
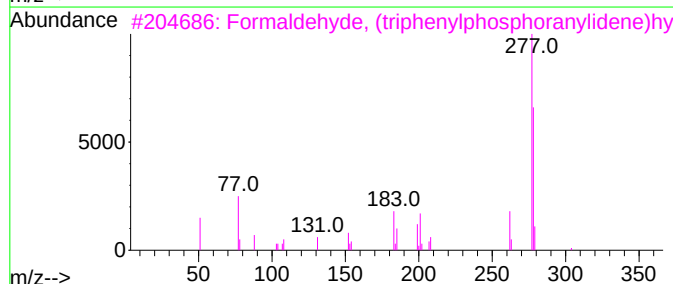
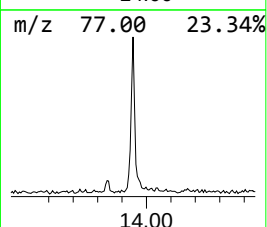
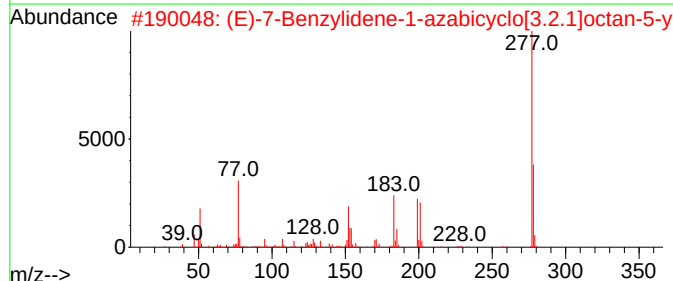
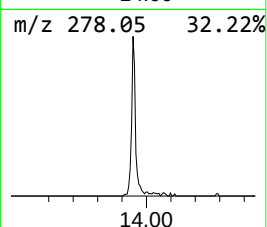
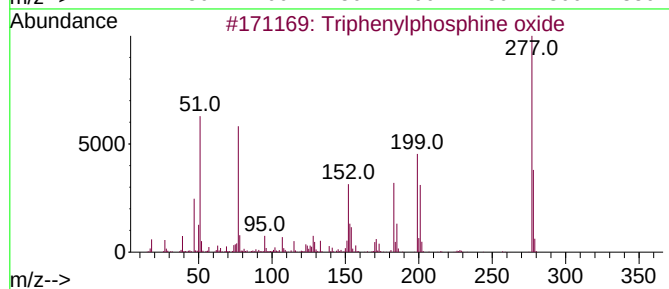
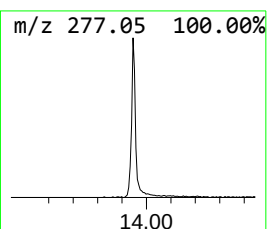
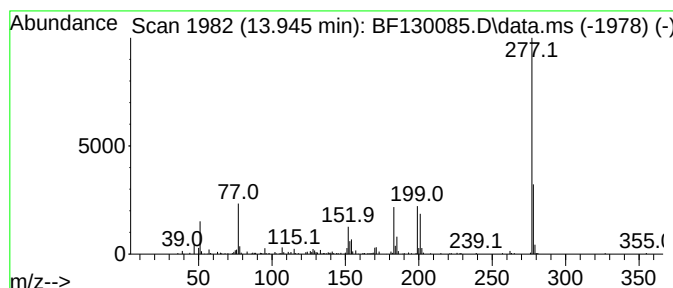
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Peak Number 4 Triphenylphosphine oxide Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.945 | 2.59 ng | 184430 | Chrysene-d12     | 13.845 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 91   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19N03S  | 1000483-83-4 | 76   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 64   |
| 4    |    |   | (Carbethoxymethyl)-triphenylphos...  | 428 | C22H22BrO2P | 001530-45-6  | 50   |
| 5    |    |   | Benzoic acid, 2-(diphenylphosphi...  | 306 | C19H15O2P   | 017261-28-8  | 38   |



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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 4.893  | 3.1     | ng    | 204702   | 1                     | 6.704  | 1299600 | 20.0 |
| Propanenitrile,... | 8.369  | 2.4     | ng    | 206355   | 2                     | 7.981  | 1743950 | 20.0 |
| 9-Octadecenoic ... | 12.322 | 3.1     | ng    | 294324   | 4                     | 11.216 | 1912790 | 20.0 |
| Triphenylphosph... | 13.945 | 2.6     | ng    | 184430   | 5                     | 13.845 | 1426370 | 20.0 |