

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062422\  
 Data File : BF128997.D  
 Acq On : 24 Jun 2022 18:58  
 Operator : CG\JU  
 Sample : N3438-01  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 FRAC-TANK-N47935

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-BF060222.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128997.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         | 3.581       | 214           | 220         | 226          | rBV      | 29534          | 50830         | 1.39%           | 0.305%        |
| 2         | 5.351       | 518           | 521         | 538          | rBV      | 1098103        | 1199895       | 32.73%          | 7.210%        |
| 3         | 6.381       | 693           | 696         | 709          | rBV      | 738769         | 725368        | 19.79%          | 4.359%        |
| 4         | 6.722       | 750           | 754         | 757          | rBV      | 722172         | 615960        | 16.80%          | 3.701%        |
| 5         | 7.257       | 840           | 845         | 847          | rBV      | 82415          | 69797         | 1.90%           | 0.419%        |
| 6         | 7.293       | 847           | 851         | 854          | rVB      | 2174825        | 2011266       | 54.86%          | 12.086%       |
| 7         | 8.004       | 968           | 972         | 976          | rVB      | 1074953        | 832205        | 22.70%          | 5.001%        |
| 8         | 8.075       | 981           | 984         | 987          | rBV      | 91795          | 81437         | 2.22%           | 0.489%        |
| 9         | 8.287       | 1017          | 1020        | 1022         | rBV      | 87083          | 66245         | 1.81%           | 0.398%        |
| 10        | 9.087       | 1148          | 1156        | 1159         | rBV      | 4298656        | 3665945       | 100.00%         | 22.028%       |
| 11        | 9.192       | 1171          | 1174        | 1180         | rVB2     | 151817         | 168365        | 4.59%           | 1.012%        |
| 12        | 9.481       | 1220          | 1223        | 1225         | rBV      | 66457          | 52883         | 1.44%           | 0.318%        |
| 13        | 9.528       | 1225          | 1231        | 1237         | rVB3     | 52012          | 104228        | 2.84%           | 0.626%        |
| 14        | 9.763       | 1267          | 1271        | 1274         | rVB      | 1003776        | 911189        | 24.86%          | 5.475%        |
| 15        | 9.834       | 1280          | 1283        | 1286         | rBV      | 43066          | 41766         | 1.14%           | 0.251%        |
| 16        | 10.369      | 1371          | 1374        | 1376         | rBV      | 54484          | 49488         | 1.35%           | 0.297%        |
| 17        | 10.392      | 1376          | 1378        | 1382         | rVV2     | 150034         | 137869        | 3.76%           | 0.828%        |
| 18        | 10.528      | 1397          | 1401        | 1402         | rBV      | 48842          | 48442         | 1.32%           | 0.291%        |
| 19        | 10.557      | 1402          | 1406        | 1409         | rVV      | 1957199        | 1766210       | 48.18%          | 10.613%       |
| 20        | 10.586      | 1409          | 1411        | 1416         | rVB      | 108262         | 95121         | 2.59%           | 0.572%        |
| 21        | 10.681      | 1421          | 1427        | 1432         | rVB5     | 60105          | 99576         | 2.72%           | 0.598%        |
| 22        | 11.245      | 1518          | 1523        | 1530         | rVB      | 618230         | 589034        | 16.07%          | 3.539%        |
| 23        | 11.639      | 1586          | 1590        | 1592         | rBV3     | 52118          | 51785         | 1.41%           | 0.311%        |
| 24        | 11.786      | 1611          | 1615        | 1622         | rBV4     | 63839          | 93611         | 2.55%           | 0.563%        |
| 25        | 12.463      | 1727          | 1730        | 1733         | rBV      | 56288          | 43481         | 1.19%           | 0.261%        |
| 26        | 12.839      | 1789          | 1794        | 1797         | rBV      | 1964056        | 1844719       | 50.32%          | 11.085%       |
| 27        | 13.445      | 1895          | 1897        | 1904         | rVB      | 46672          | 44337         | 1.21%           | 0.266%        |
| 28        | 13.745      | 1944          | 1948        | 1958         | rBV3     | 52440          | 122055        | 3.33%           | 0.733%        |
| 29        | 13.892      | 1970          | 1973        | 1982         | rVB      | 515462         | 457609        | 12.48%          | 2.750%        |
| 30        | 13.992      | 1984          | 1990        | 1995         | rBV      | 145792         | 169643        | 4.63%           | 1.019%        |
| 31        | 15.333      | 2213          | 2218        | 2227         | rVB      | 366936         | 431495        | 11.77%          | 2.593%        |

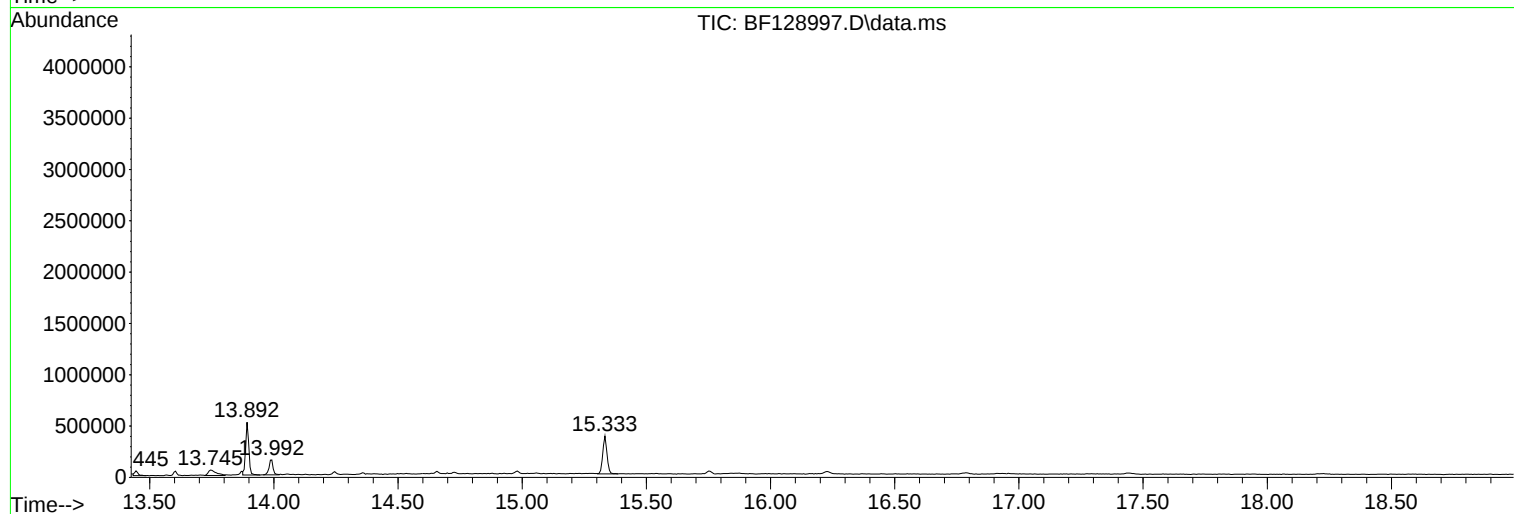
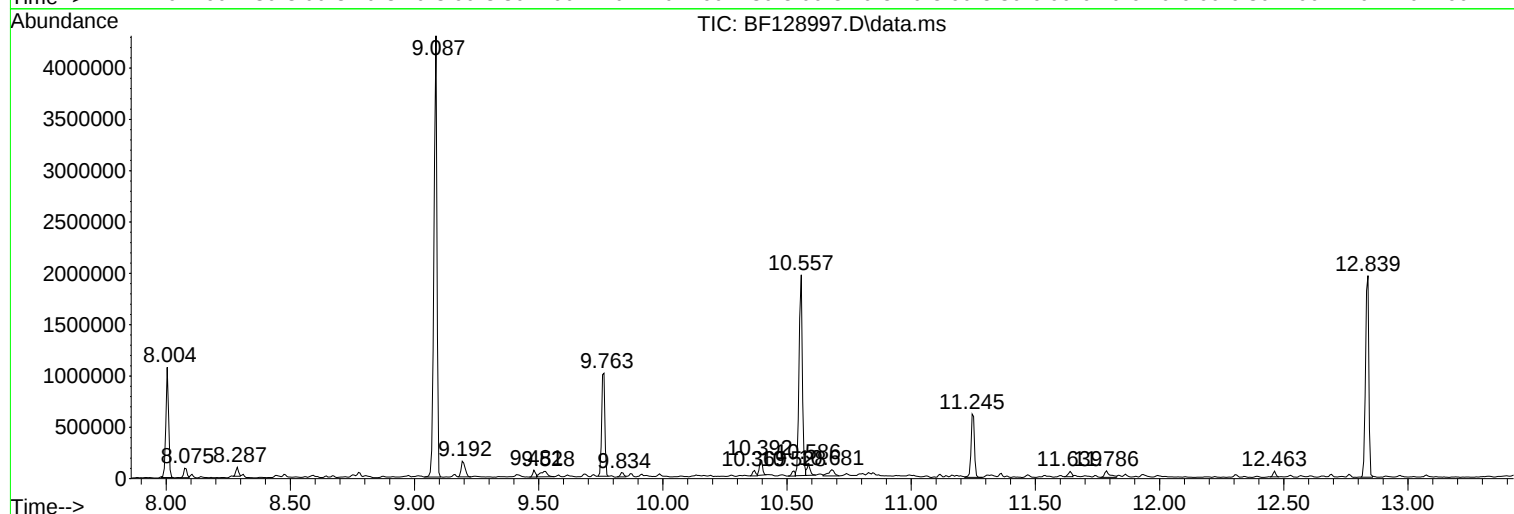
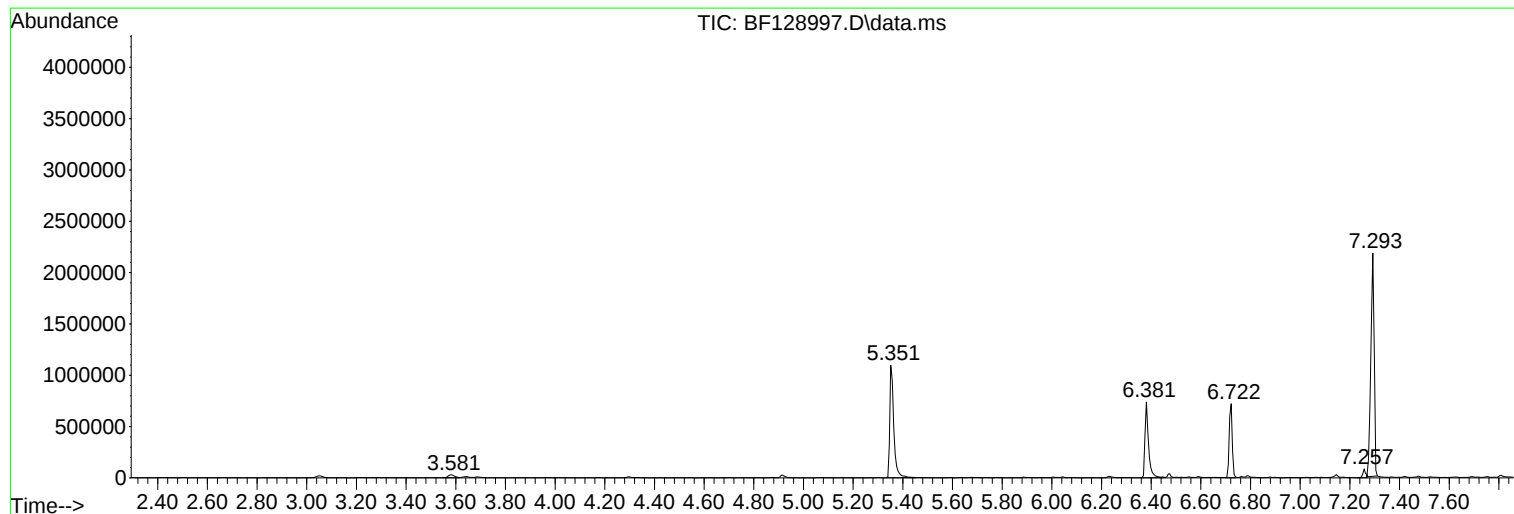
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ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
FRAC-TANK-N47935

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.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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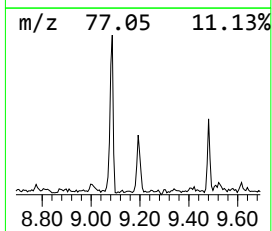
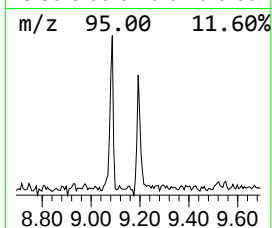
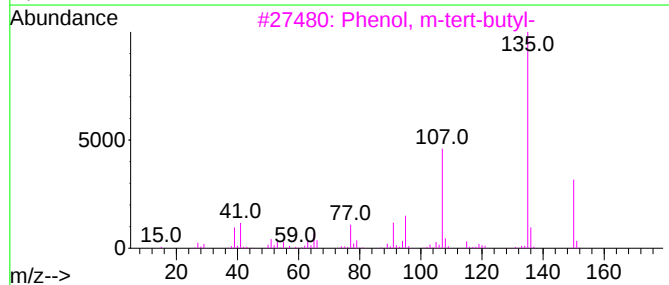
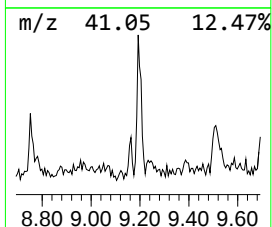
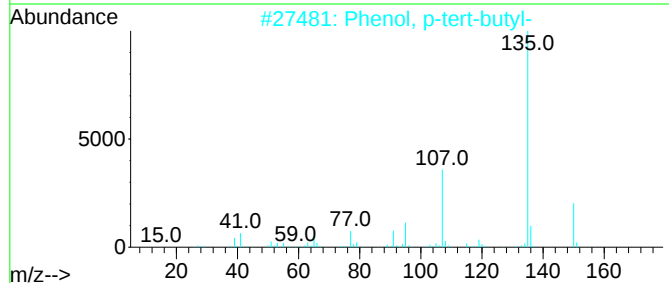
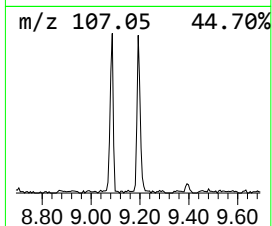
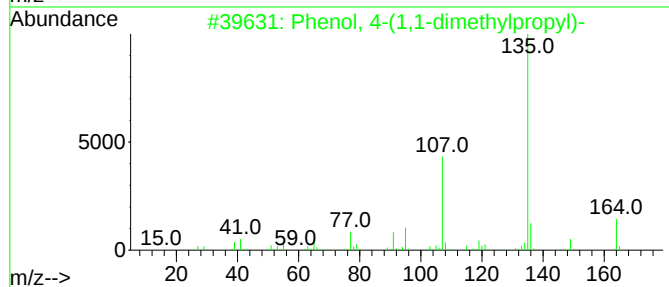
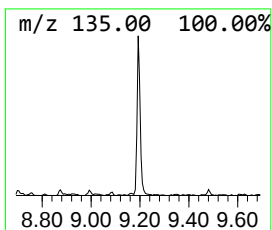
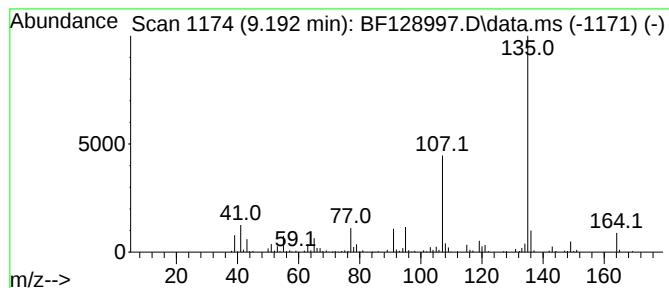
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Phenol, 4-(1,1-dimethylprop... Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 9.192 | 3.70 ng | 168365 | Acenaphthene-d10 | 9.763 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Phenol, 4-(1,1-dimethylpropyl)-     | 164 | C11H16O    | 000080-46-6  | 96   |
| 2    |    |   | Phenol, p-tert-butyl-               | 150 | C10H14O    | 000098-54-4  | 78   |
| 3    |    |   | Phenol, m-tert-butyl-               | 150 | C10H14O    | 000585-34-2  | 78   |
| 4    |    |   | Hexestrol, 0-heptafluorobutyryl-    | 466 | C22H21F7O3 | 1000365-31-9 | 64   |
| 5    |    |   | Phenol, 4-(1,1,3,3-tetramethylbu... | 206 | C14H22O    | 000140-66-9  | 64   |



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FRAC-TANK-N47935

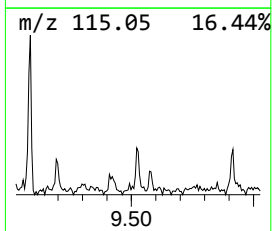
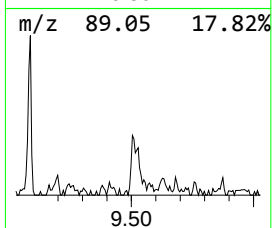
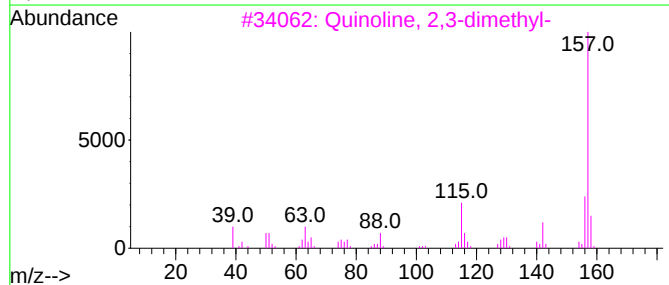
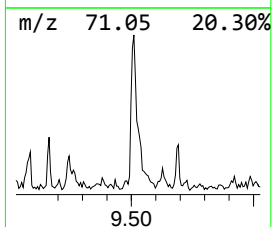
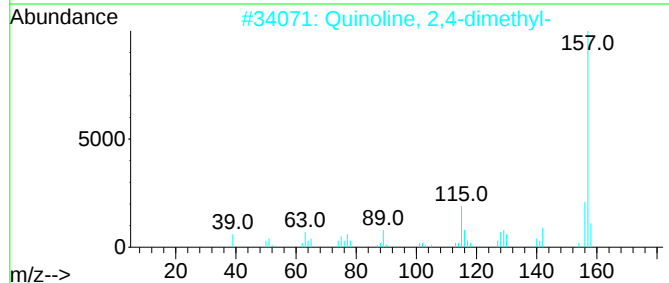
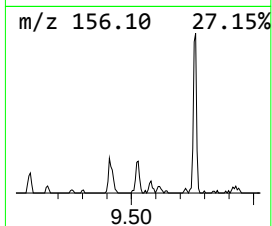
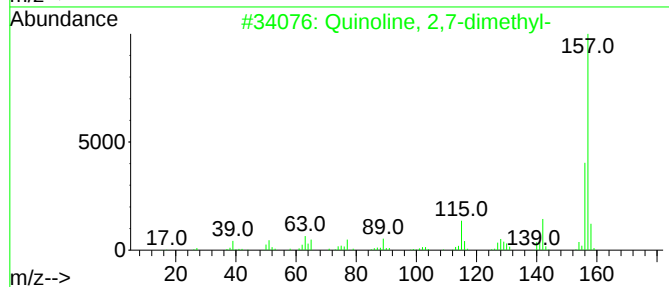
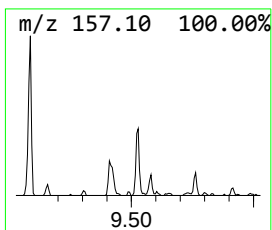
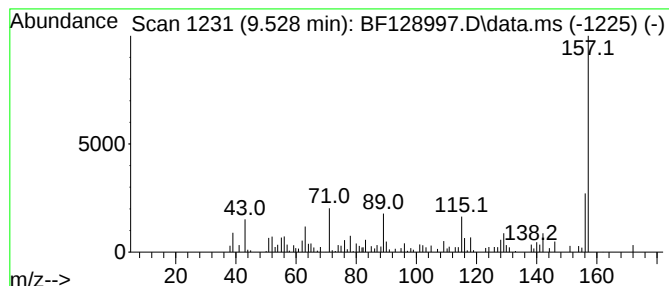
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Quinoline, 2,7-dimethyl- Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 9.528 | 2.29 ng | 104228 | Acenaphthene-d10 | 9.763 |

| Hit# | of 5 | Tentative ID             | MW  | MolForm | CAS#        | Qual |
|------|------|--------------------------|-----|---------|-------------|------|
| 1    |      | Quinoline, 2,7-dimethyl- | 157 | C11H11N | 000093-37-8 | 93   |
| 2    |      | Quinoline, 2,4-dimethyl- | 157 | C11H11N | 001198-37-4 | 70   |
| 3    |      | Quinoline, 2,3-dimethyl- | 157 | C11H11N | 001721-89-7 | 58   |
| 4    |      | Quinoline, 4-ethyl-      | 157 | C11H11N | 019020-26-9 | 58   |
| 5    |      | Quinoline, 2,6-dimethyl- | 157 | C11H11N | 000877-43-0 | 53   |



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Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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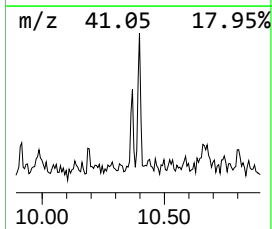
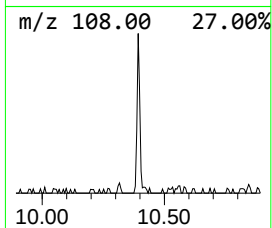
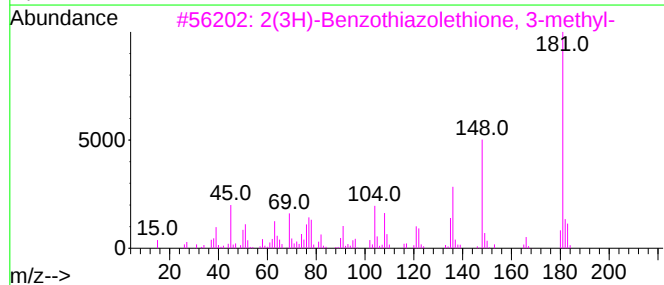
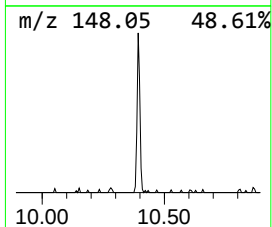
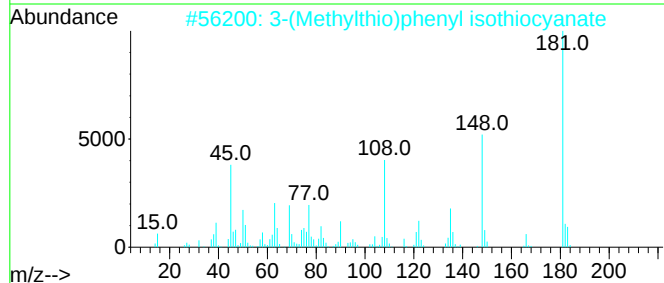
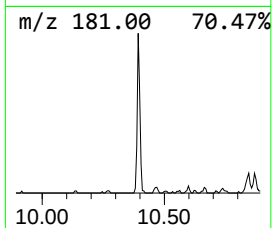
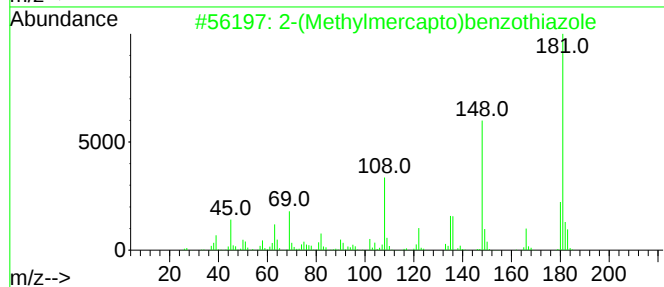
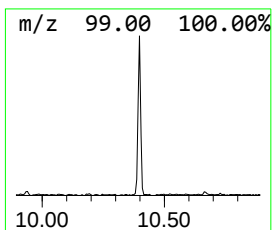
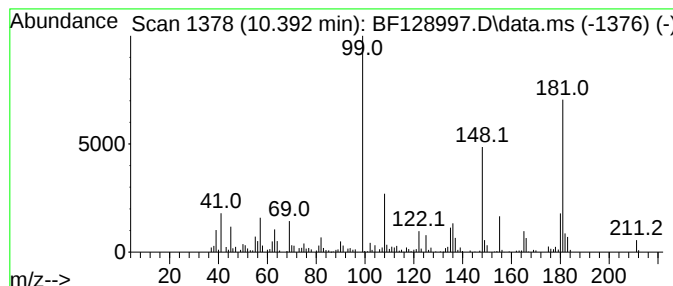
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 2-(Methylmercapto)benzothia... Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.  |
|--------|---------|--------|------------------|-------|
| 10.392 | 3.03 ng | 137869 | Acenaphthene-d10 | 9.763 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | 2-(Methylmercapto)benzothiazole     | 181 | C8H7NS2   | 000615-22-5 | 96   |
| 2    |    |   | 3-(Methylthio)phenyl isothiocyanate | 181 | C8H7NS2   | 051333-80-3 | 50   |
| 3    |    |   | 2(3H)-Benzothiazolethione, 3-met... | 181 | C8H7NS2   | 002254-94-6 | 35   |
| 4    |    |   | 4-(Methylthio)phenyl isothiocyanate | 181 | C8H7NS2   | 015863-41-9 | 35   |
| 5    |    |   | Triisobutyl phosphate               | 266 | C12H27O4P | 000126-71-6 | 22   |



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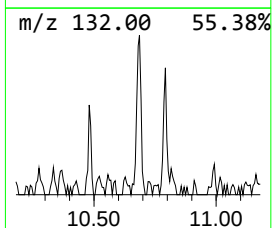
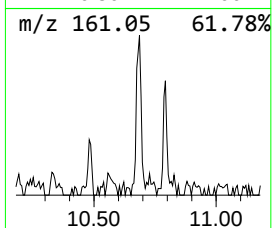
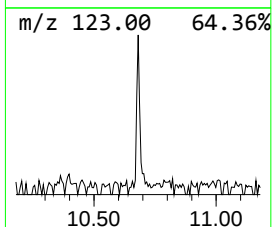
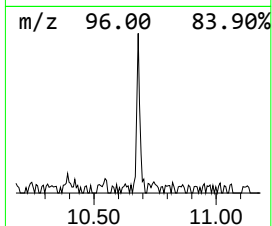
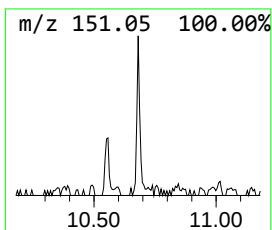
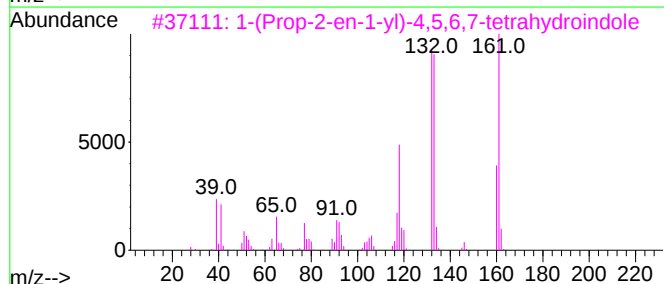
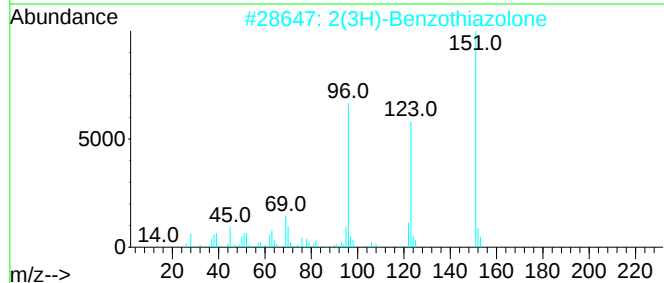
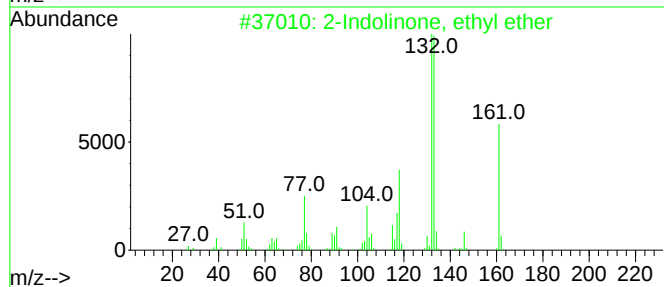
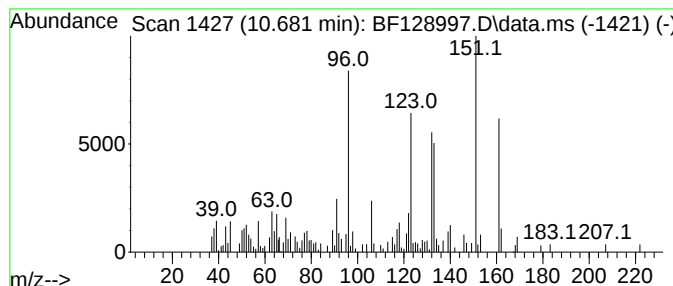
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 unknown10.681 Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 10.681 | 3.38 ng | 99576 | Phenanthrene-d10 | 11.245 |

| Hit# | of                                  | 5 | Tentative ID | MW       | MolForm      | CAS# | Qual |
|------|-------------------------------------|---|--------------|----------|--------------|------|------|
| 1    | 2-Indolinone, ethyl ether           |   | 161          | C10H11NO | 1000453-17-4 | 47   |      |
| 2    | 2(3H)-Benzothiazolone               |   | 151          | C7H5NOS  | 000934-34-9  | 43   |      |
| 3    | 1-(Prop-2-en-1-yl)-4,5,6,7-tetra... |   | 161          | C11H15N  | 1450892-88-2 | 38   |      |
| 4    | 2-Amino-5-methylbenzoic acid        |   | 151          | C8H9NO2  | 002941-78-8  | 22   |      |
| 5    | 4,6-Dimethylpyridine-3-carboxyli... |   | 151          | C8H9NO2  | 022047-86-5  | 22   |      |



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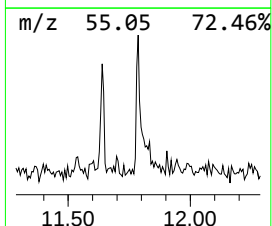
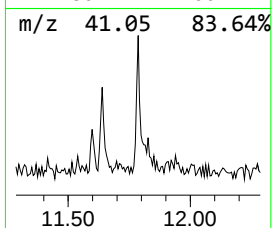
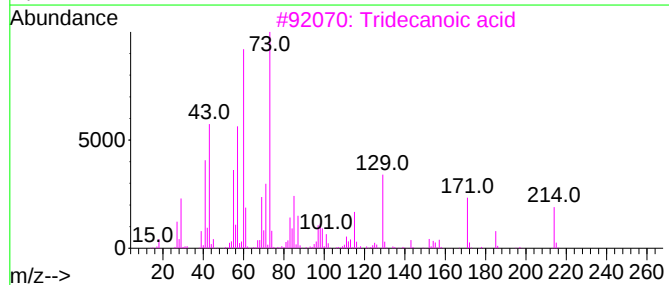
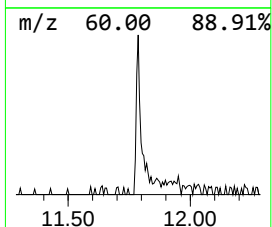
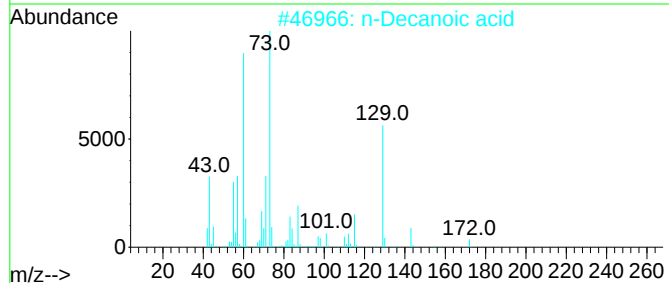
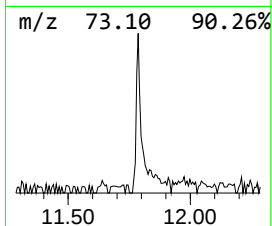
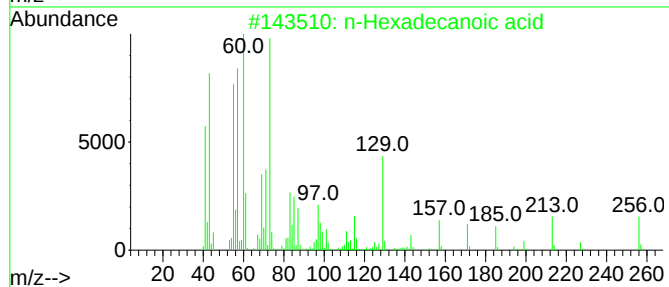
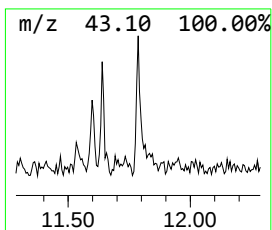
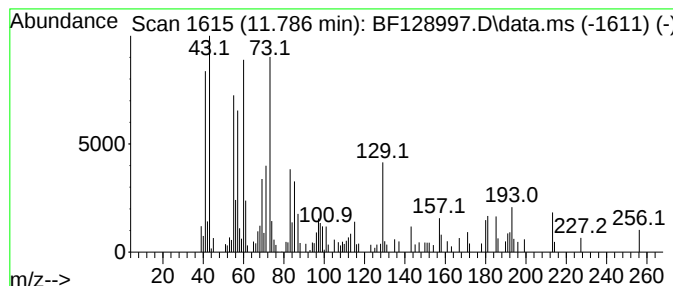
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.786 | 3.18 ng | 93611 | Phenanthrene-d10 | 11.245 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97   |
| 2    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 87   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 78   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 62   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062422\  
Data File : BF128997.D  
Acq On : 24 Jun 2022 18:58  
Operator : CG\JU  
Sample : N3438-01  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
FRAC-TANK-N47935

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

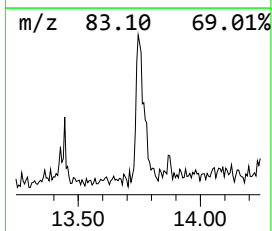
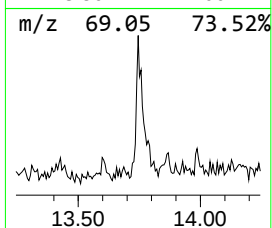
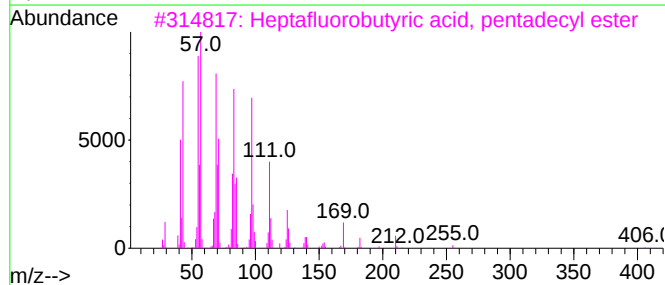
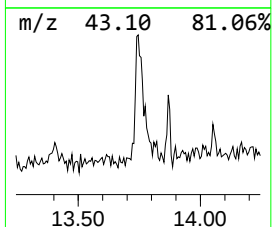
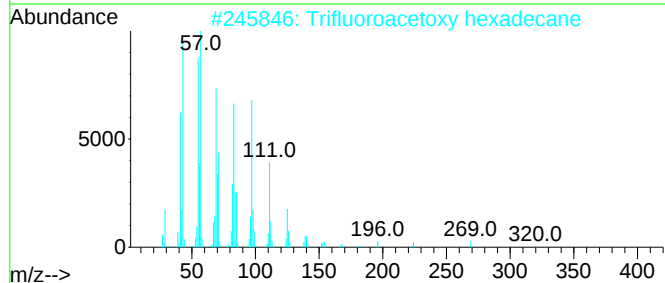
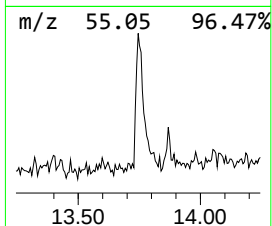
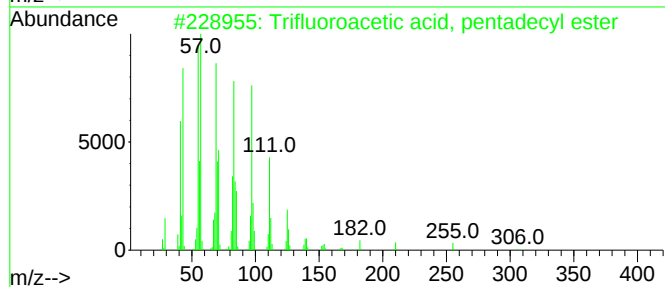
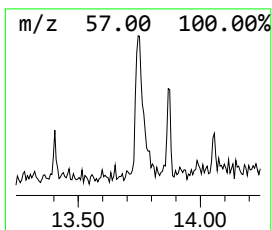
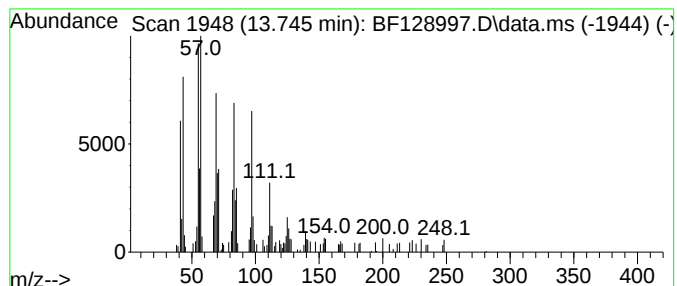
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Trifluoroacetic acid, penta... Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.745 | 5.33 ng | 122055 | Chrysene-d12     | 13.892 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2  | 95   |
| 2    |    |   | Trifluoroacetoxy hexadecane         | 338 | C18H33F3O2 | 006222-03-3  | 95   |
| 3    |    |   | Heptafluorobutyric acid, pentade... | 424 | C19H31F7O2 | 959261-23-5  | 95   |
| 4    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1  | 94   |
| 5    |    |   | Heptadecyl trifluoroacetate         | 352 | C19H35F3O2 | 1010351-87-0 | 93   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062422\  
Data File : BF128997.D  
Acq On : 24 Jun 2022 18:58  
Operator : CG\JU  
Sample : N3438-01  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
FRAC-TANK-N47935

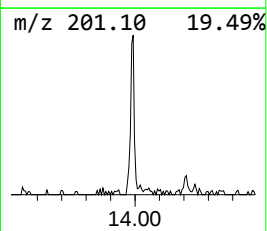
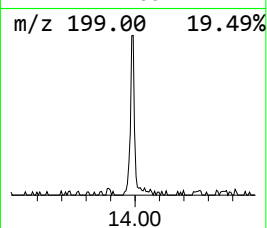
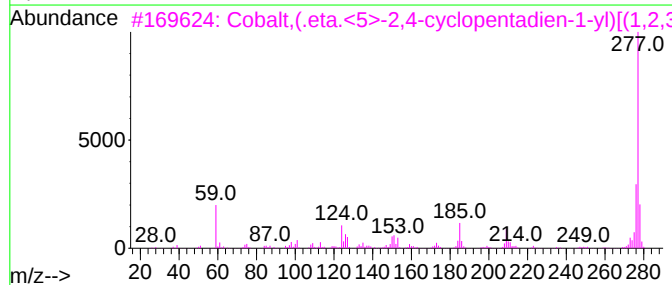
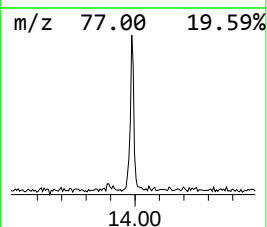
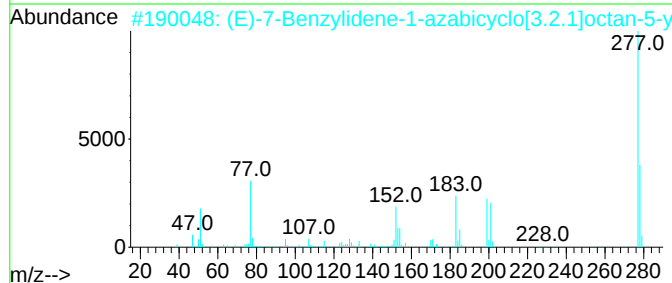
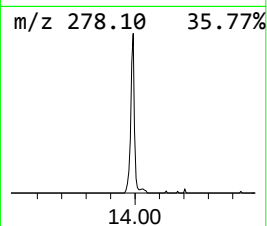
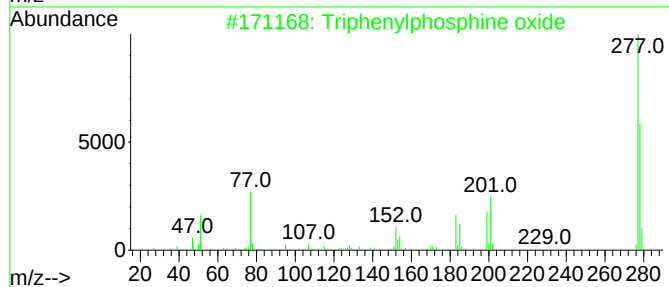
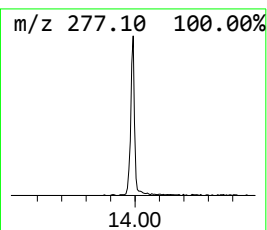
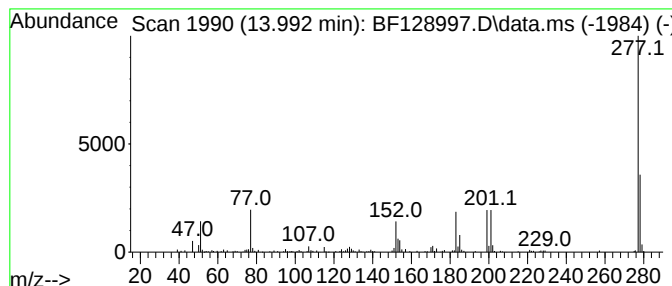
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.992 | 7.41 ng | 169643 | Chrysene-d12     | 13.892 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 93   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S | 1000483-83-4 | 81   |
| 3    |    |   | Cobalt,(.eta.<5>-2,4-cyclopentad...  | 277 | C16H15BCo  | 036682-12-9  | 38   |
| 4    |    |   | 5-Methyl-8-phenylfuro[3',2':5,6]...  | 277 | C16H11N3O2 | 1000460-07-9 | 38   |
| 5    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 25   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF062422\  
Data File : BF128997.D  
Acq On : 24 Jun 2022 18:58  
Operator : CG\JU  
Sample : N3438-01  
Misc :  
ALS Vial : 19 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
FRAC-TANK-N47935

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| Phenol, 4-(1,1-... | 9.192  | 3.7     | ng    | 168365   | 3                     | 9.763  | 911189 | 20.0 |
| Quinoline, 2,7-... | 9.528  | 2.3     | ng    | 104228   | 3                     | 9.763  | 911189 | 20.0 |
| 2-(Methylmercap... | 10.392 | 3.0     | ng    | 137869   | 3                     | 9.763  | 911189 | 20.0 |
| unknown10.681      | 10.681 | 3.4     | ng    | 99576    | 4                     | 11.245 | 589034 | 20.0 |
| n-Hexadecanoic ... | 11.786 | 3.2     | ng    | 93611    | 4                     | 11.245 | 589034 | 20.0 |
| Trifluoroacetic... | 13.745 | 5.3     | ng    | 122055   | 5                     | 13.892 | 457609 | 20.0 |
| Triphenylphosph... | 13.992 | 7.4     | ng    | 169643   | 5                     | 13.892 | 457609 | 20.0 |