

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
 Data File : BP008789.D  
 Acq On : 13 Jan 2022 14:37  
 Operator : CG/JU  
 Sample : N1098-03  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 14-G-WATER

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-BP010622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP008789.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         | 3.064       | 8             | 13          | 35           | rVB      | 8037350        | 9893182       | 34.77%          | 9.078%        |
| 2         | 5.446       | 412           | 418         | 437          | rBV      | 2369834        | 3763899       | 13.23%          | 3.454%        |
| 3         | 7.040       | 680           | 689         | 705          | rBV      | 1274688        | 2342091       | 8.23%           | 2.149%        |
| 4         | 7.863       | 822           | 829         | 837          | rBV      | 1066627        | 1763573       | 6.20%           | 1.618%        |
| 5         | 9.028       | 1018          | 1027        | 1049         | rBV      | 3090788        | 5503112       | 19.34%          | 5.049%        |
| 6         | 10.457      | 1261          | 1270        | 1286         | rBV      | 156081         | 388186        | 1.36%           | 0.356%        |
| 7         | 10.669      | 1298          | 1306        | 1322         | rBV      | 1264442        | 2274382       | 7.99%           | 2.087%        |
| 8         | 12.134      | 1543          | 1555        | 1562         | rBV      | 157723         | 304779        | 1.07%           | 0.280%        |
| 9         | 13.128      | 1717          | 1724        | 1742         | rBV      | 8777932        | 13253042      | 46.58%          | 12.160%       |
| 10        | 14.504      | 1951          | 1958        | 1976         | rBV      | 1822627        | 2905636       | 10.21%          | 2.666%        |
| 11        | 15.998      | 2205          | 2212        | 2234         | rBV      | 5956911        | 9304304       | 32.70%          | 8.537%        |
| 12        | 17.257      | 2420          | 2426        | 2440         | rBV      | 2036945        | 3226695       | 11.34%          | 2.961%        |
| 13        | 18.151      | 2574          | 2578        | 2586         | rBV      | 327961         | 564871        | 1.99%           | 0.518%        |
| 14        | 19.822      | 2856          | 2862        | 2872         | rBV      | 13283950       | 16534800      | 58.11%          | 15.172%       |
| 15        | 19.922      | 2873          | 2879        | 2893         | rBV2     | 209015         | 815451        | 2.87%           | 0.748%        |
| 16        | 21.057      | 3069          | 3072        | 3080         | rBV2     | 686978         | 933727        | 3.28%           | 0.857%        |
| 17        | 21.345      | 3117          | 3121        | 3129         | rBV      | 2545770        | 3353395       | 11.79%          | 3.077%        |
| 18        | 21.469      | 3136          | 3142        | 3168         | rBV      | 17363816       | 28452090      | 100.00%         | 26.106%       |
| 19        | 23.774      | 3528          | 3534        | 3545         | rVB2     | 1596928        | 3407724       | 11.98%          | 3.127%        |

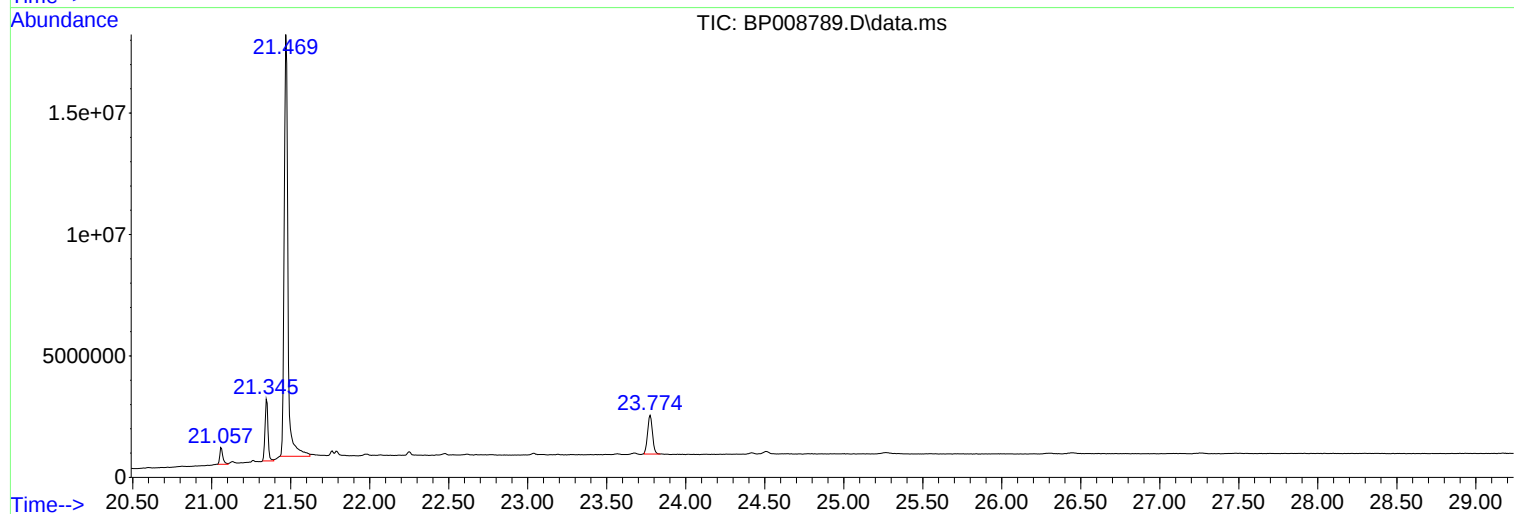
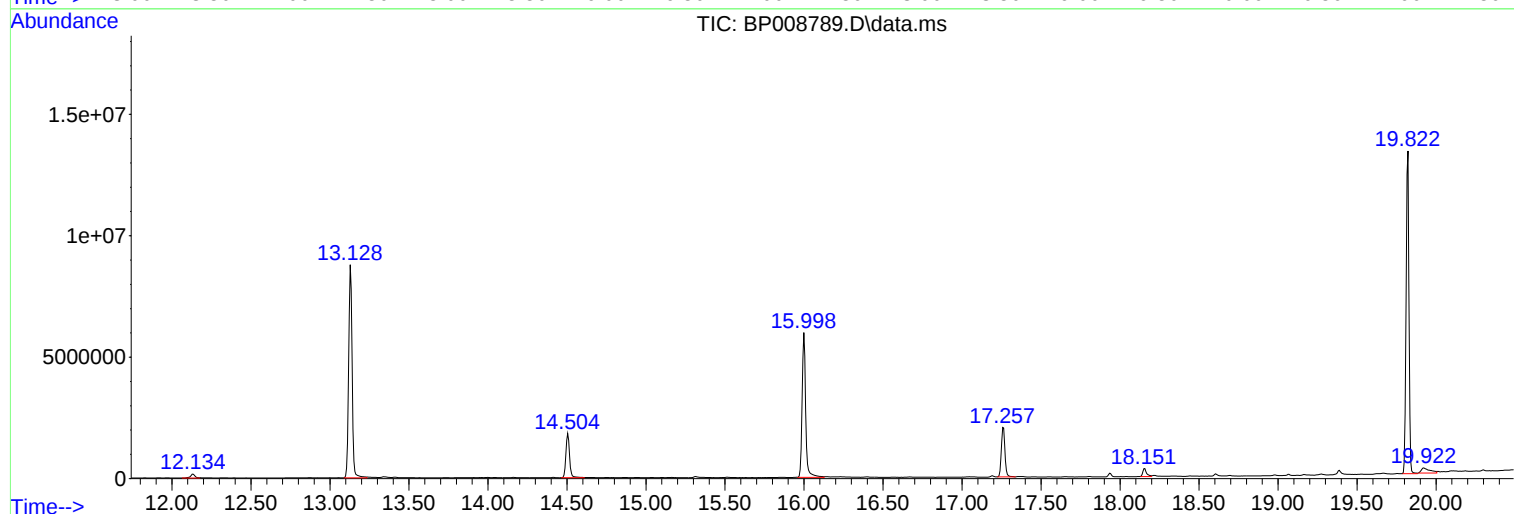
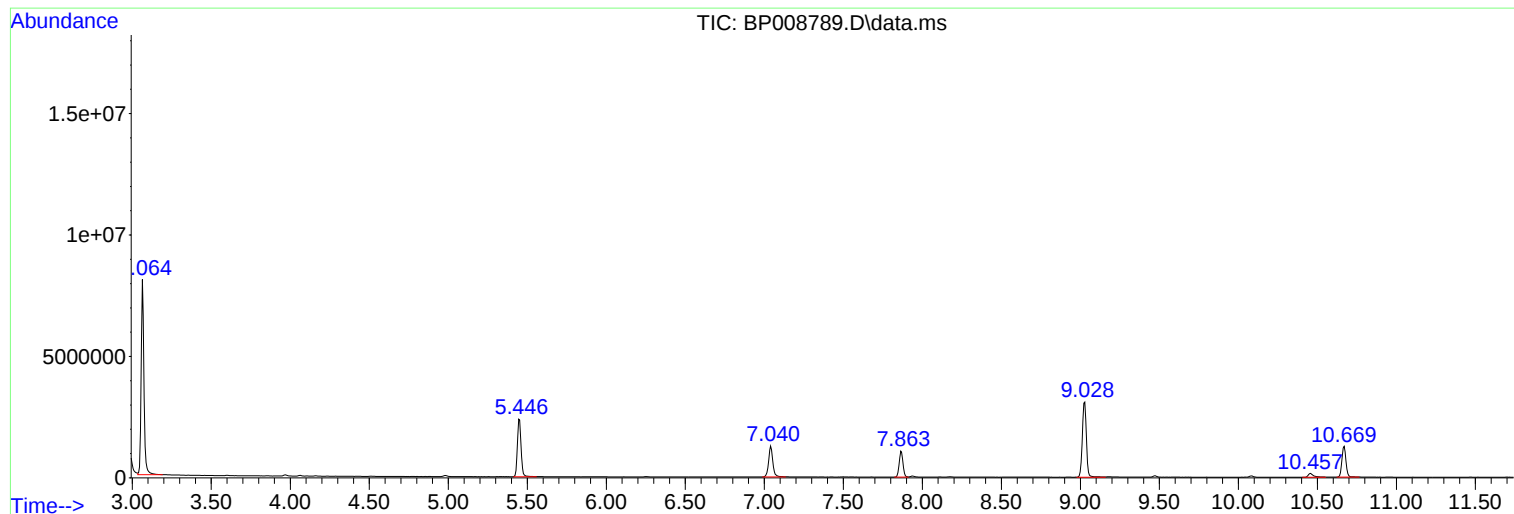
Sum of corrected areas: 108984939

Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

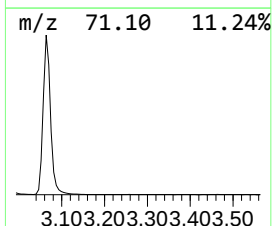
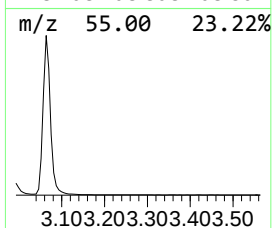
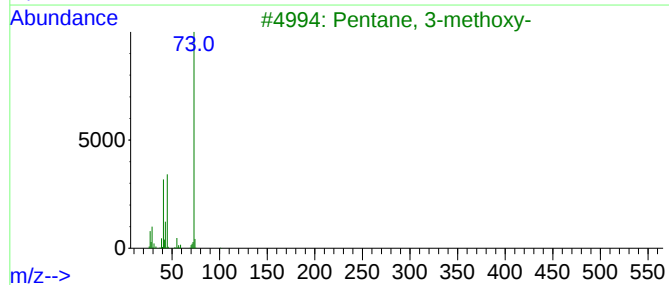
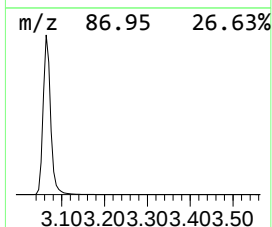
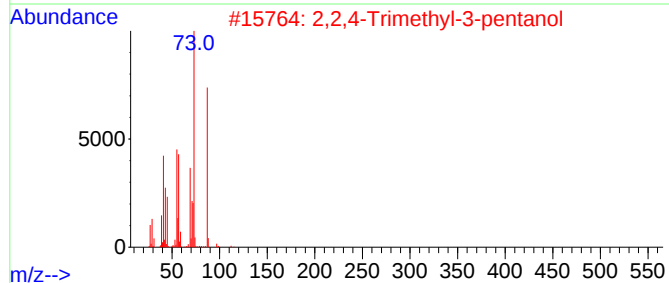
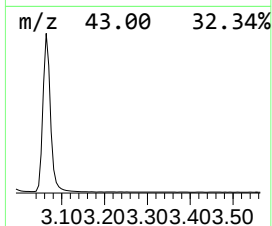
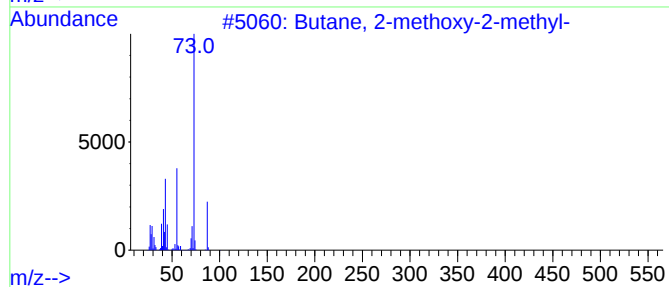
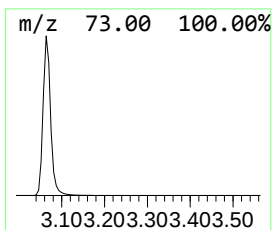
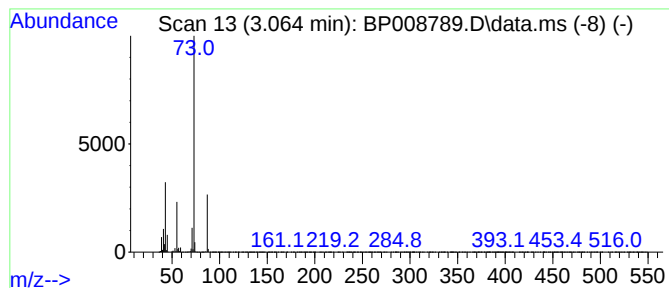
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 2

| R.T.  | EstConc   | Area    | Relative to ISTD       | R.T.  |
|-------|-----------|---------|------------------------|-------|
| 3.064 | 112.19 ng | 9893180 | 1,4-Dichlorobenzene-d4 | 7.863 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------|-----|---------|-------------|------|
| 1    |    |   | Butane, 2-methoxy-2-methyl- | 102 | C6H14O  | 000994-05-8 | 83   |
| 2    |    |   | 2,2,4-Trimethyl-3-pentanol  | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    |   | Pentane, 3-methoxy-         | 102 | C6H14O  | 036839-67-5 | 23   |
| 4    |    |   | Acetamide, N-ethyl-         | 87  | C4H9NO  | 000625-50-3 | 9    |
| 5    |    |   | Silane, tetramethyl-        | 88  | C4H12Si | 000075-76-3 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

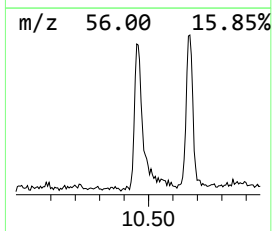
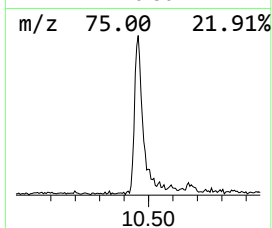
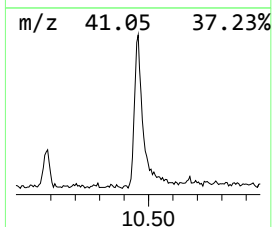
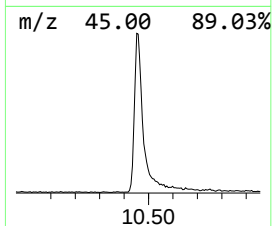
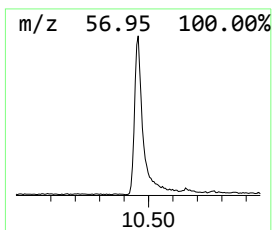
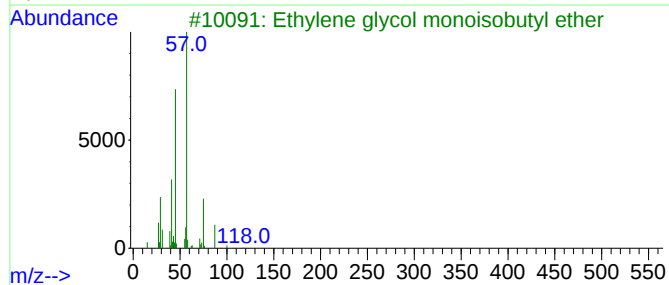
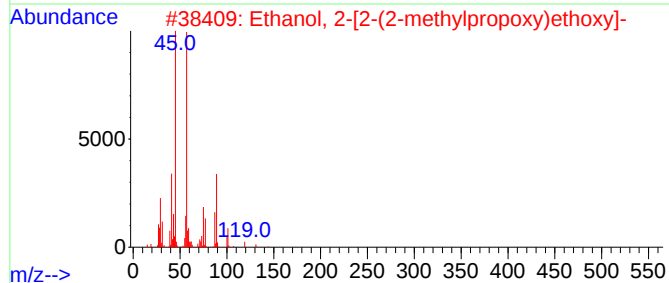
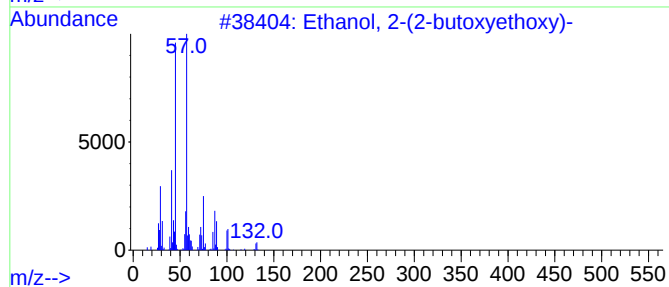
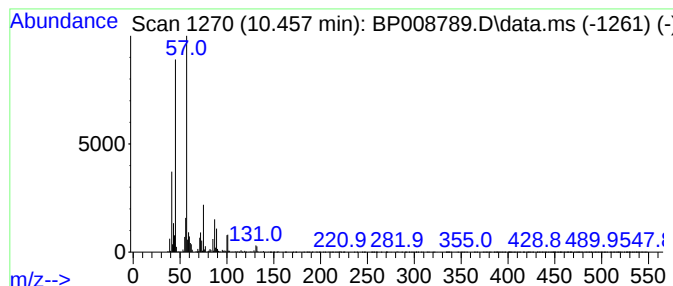
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 Ethanol, 2-(2-butoxyethoxy)- Concentration Rank 6

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.457 | 3.41 ng | 388186 | Naphthalene-d8   | 10.669 |

| Hit# | of | 5 | Tentative ID                            | MW  | MolForm | CAS#        | Qual |
|------|----|---|-----------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Ethanol, 2-(2-butoxyethoxy)-            | 162 | C8H18O3 | 000112-34-5 | 91   |
| 2    |    |   | Ethanol, 2-[2-(2-methylpropoxy)ethoxy]- | 162 | C8H18O3 | 018912-80-6 | 64   |
| 3    |    |   | Ethylene glycol monoisobutyl ether      | 118 | C6H14O2 | 004439-24-1 | 59   |
| 4    |    |   | Ethanol, 1-(2-butoxyethoxy)-            | 162 | C8H18O3 | 054446-78-5 | 50   |
| 5    |    |   | 3,3-Dimethylbutane-2-ol                 | 102 | C6H14O  | 000464-07-3 | 50   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

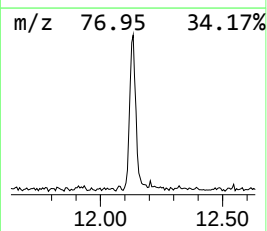
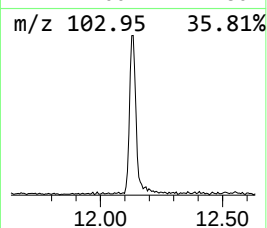
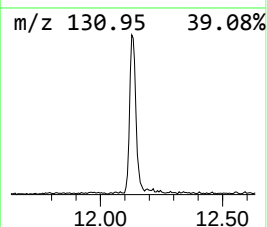
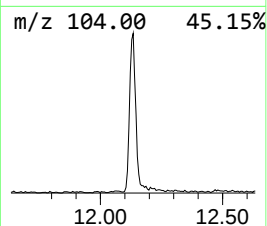
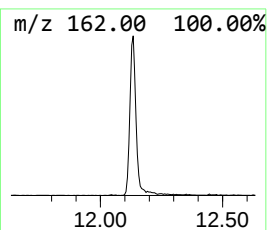
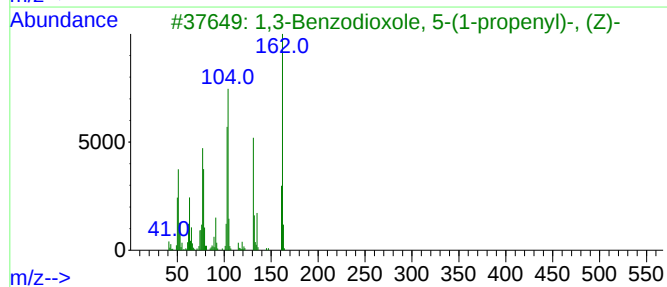
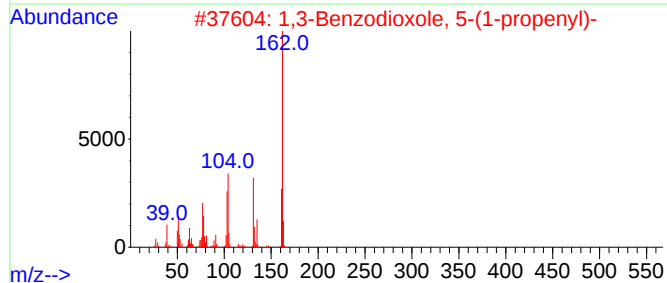
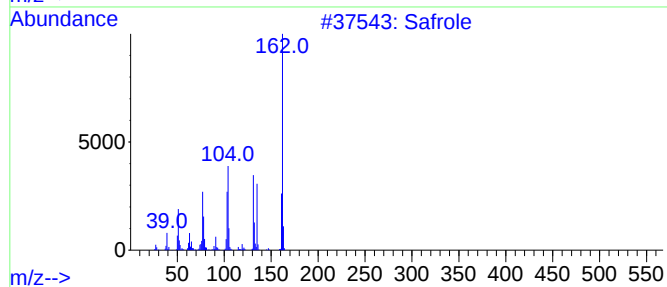
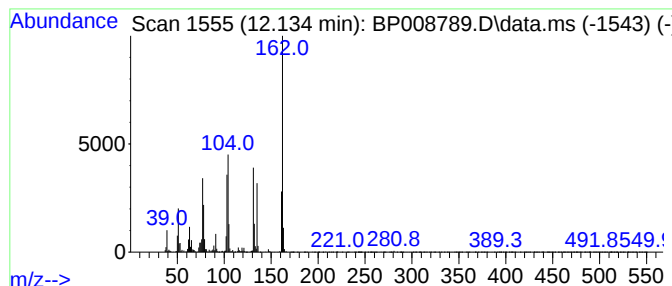
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 Safole Concentration Rank 7

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 12.134 | 2.68 ng | 304779 | Naphthalene-d8   | 10.669 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|----------|--------------|------|
| 1    |    |   | Safole                               | 162 | C10H10O2 | 000094-59-7  | 98   |
| 2    |    |   | 1,3-Benzodioxole, 5-(1-propenyl)-    | 162 | C10H10O2 | 000120-58-1  | 97   |
| 3    |    |   | 1,3-Benzodioxole, 5-(1-propenyl)-... | 162 | C10H10O2 | 017627-76-8  | 97   |
| 4    |    |   | Benzene, 1,2-(methylenedioxy)-4-...  | 162 | C10H10O2 | 004043-71-4  | 97   |
| 5    |    |   | 3-pyrazolidinone, 5-phenyl-          | 162 | C9H10N2O | 1000404-42-6 | 59   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

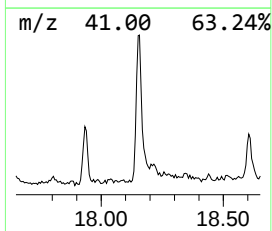
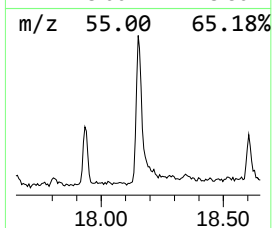
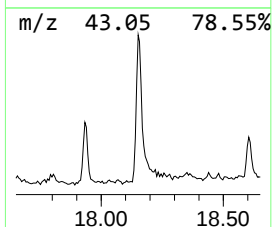
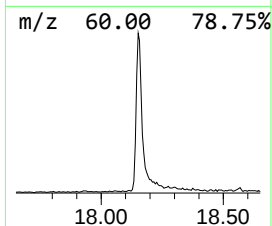
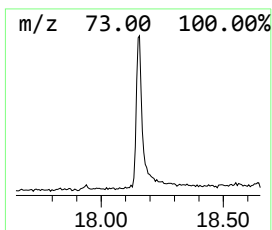
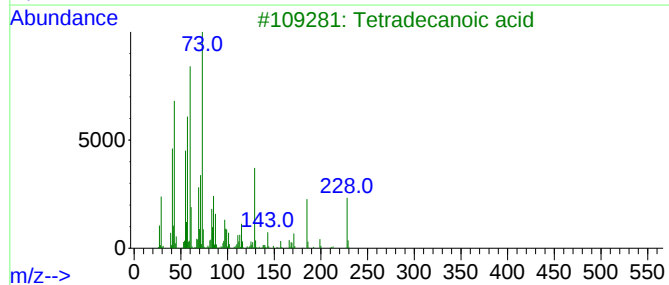
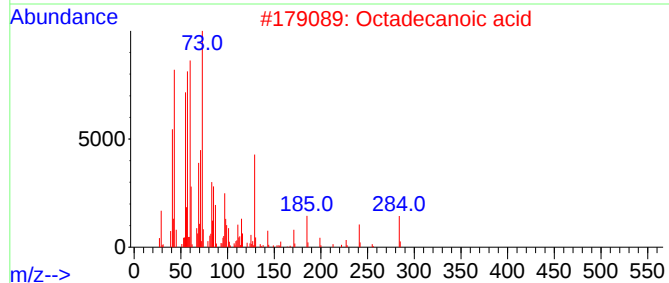
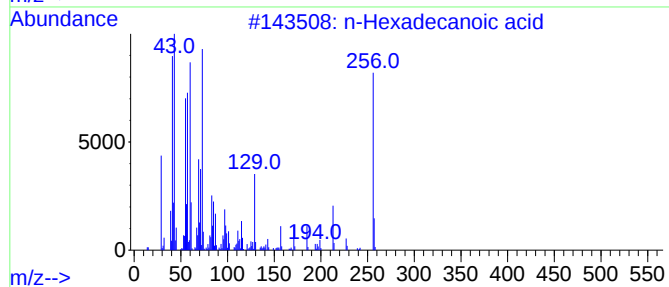
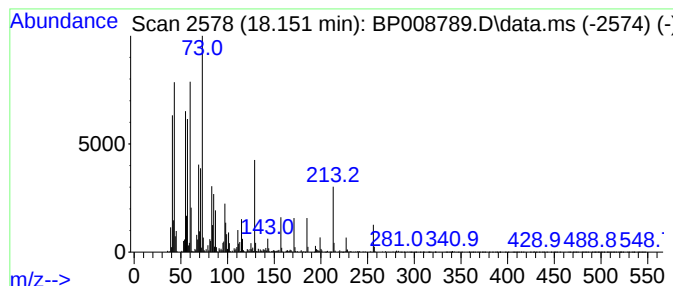
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 18.151 | 3.50 ng | 564871 | Phenanthrene-d10 | 17.257 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 93   |
| 3    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 91   |
| 4    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 5    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 90   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

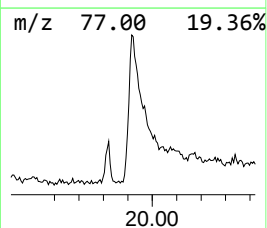
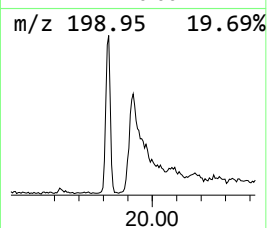
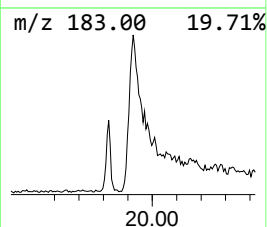
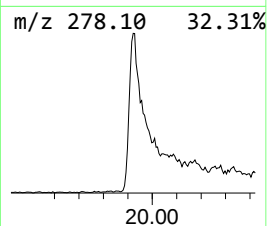
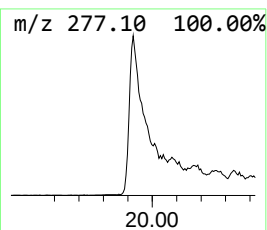
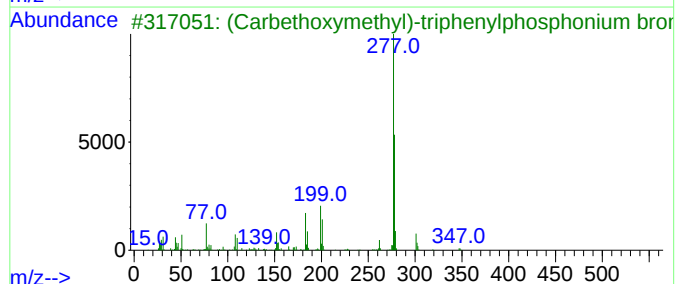
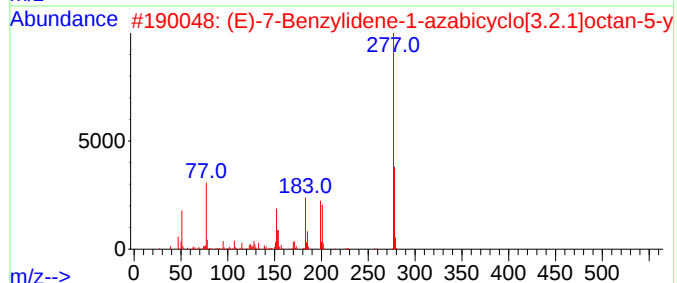
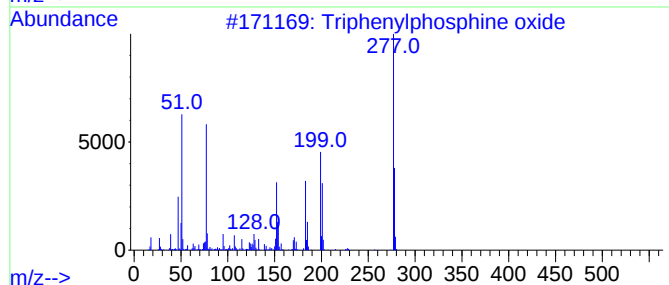
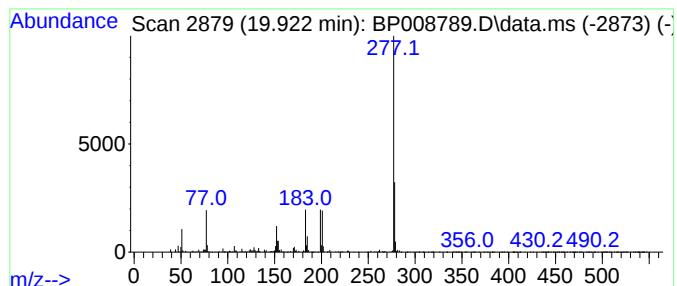
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 Triphenylphosphine oxide Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.922 | 4.86 ng | 815451 | Chrysene-d12     | 21.345 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm     | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP    | 000791-28-6  | 83   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S  | 1000483-83-4 | 72   |
| 3    |    |   | (Carbethoxymethyl)-triphenylphos...  | 428 | C22H22BrO2P | 001530-45-6  | 45   |
| 4    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P   | 015990-54-2  | 42   |
| 5    |    |   | 5-Methyl-8-phenylfuro[3',2':5,6]...  | 277 | C16H11N3O2  | 1000460-07-9 | 37   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

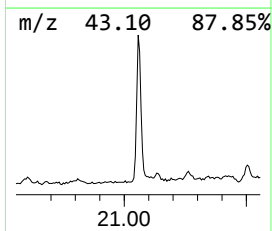
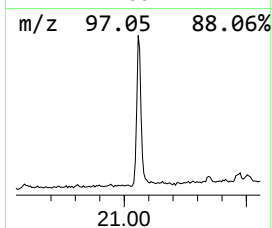
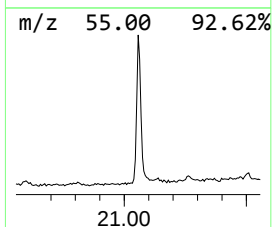
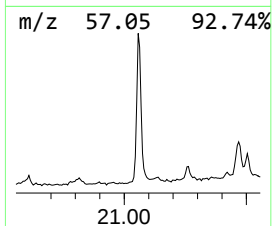
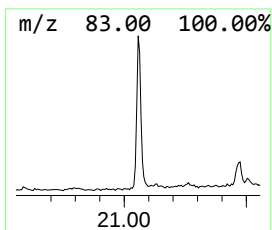
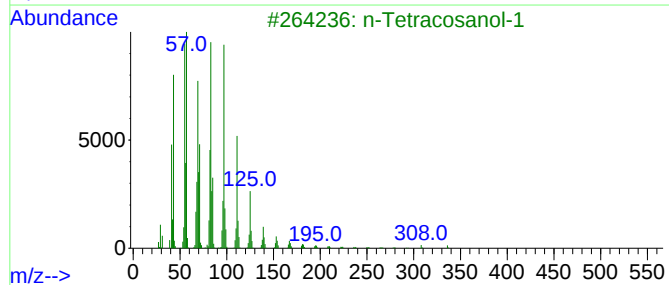
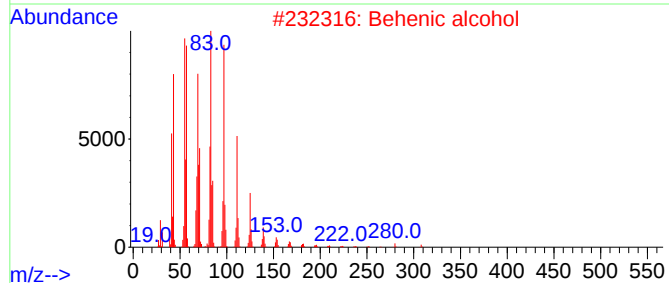
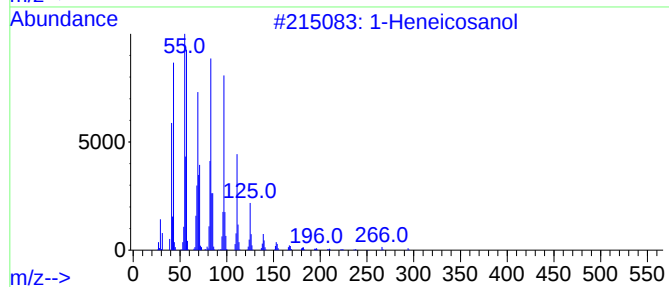
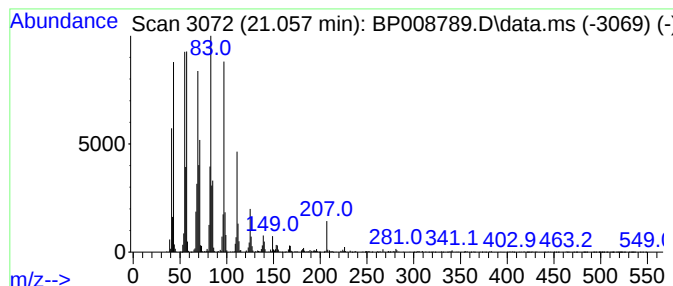
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 1-Heneicosanol Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 21.057 | 5.57 ng | 933727 | Chrysene-d12     | 21.345 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|------------|-------------|------|
| 1    |    |   | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 95   |
| 2    |    |   | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 95   |
| 3    |    |   | n-Tetracosanol-1                    | 354 | C24H50O    | 000506-51-4 | 95   |
| 4    |    |   | 1-Heptacosanol                      | 396 | C27H56O    | 002004-39-9 | 94   |
| 5    |    |   | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 94   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
Data File : BP008789.D  
Acq On : 13 Jan 2022 14:37  
Operator : CG/JU  
Sample : N1098-03  
Misc :  
ALS Vial : 5 Sample Multiplier: 1

Instrument :  
BNA\_P  
ClientSampleId :  
14-G-WATER

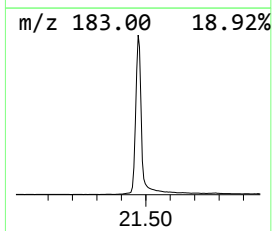
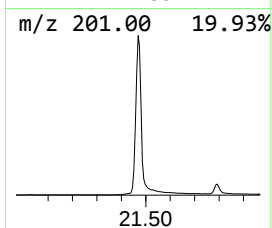
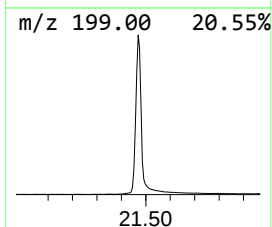
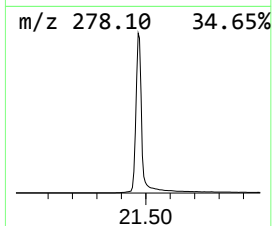
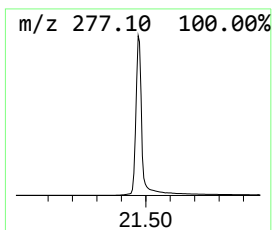
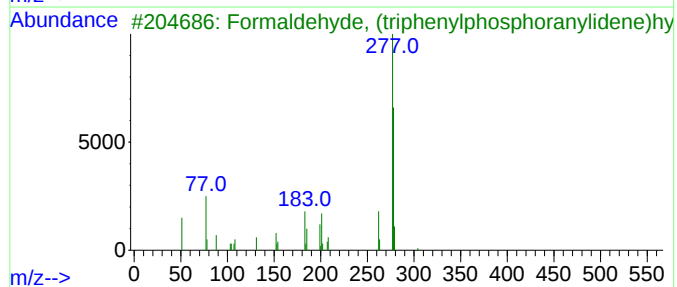
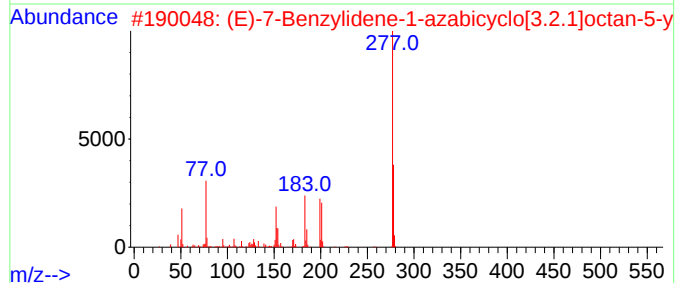
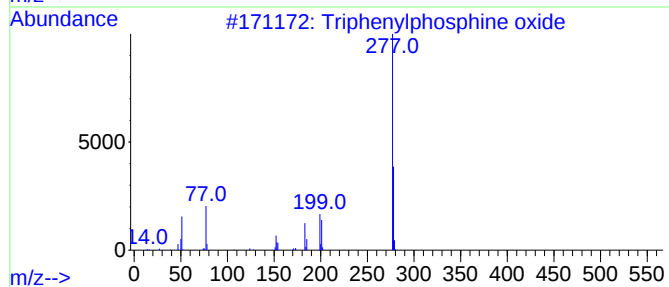
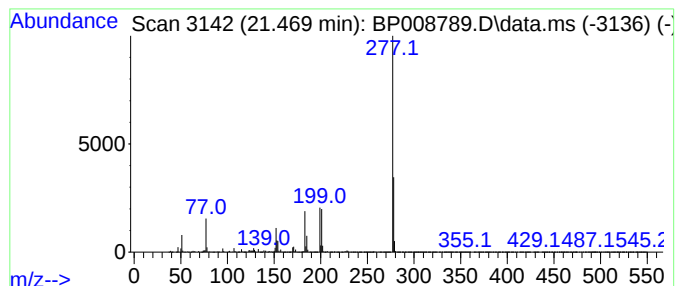
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 7 unknown21.469 Concentration Rank 1

| R.T.   | EstConc   | Area     | Relative to ISTD | R.T.   |
|--------|-----------|----------|------------------|--------|
| 21.469 | 169.69 ng | 28452100 | Chrysene-d12     | 21.345 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|------|----|---|--------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Triphenylphosphine oxide             | 278 | C18H15OP   | 000791-28-6  | 96   |
| 2    |    |   | (E)-7-Benzylidene-1-azabicyclo[3...] | 293 | C15H19NO3S | 1000483-83-4 | 80   |
| 3    |    |   | Formaldehyde, (triphenylphosphor...  | 304 | C19H17N2P  | 015990-54-2  | 45   |
| 4    |    |   | 5-Methyl-8-phenylfuro[3',2':5,6]...  | 277 | C16H11N3O2 | 1000460-07-9 | 25   |
| 5    |    |   | [1,2,4]Triazolo[1,5-a]pyrimidine...  | 278 | C15H14N6   | 1000350-69-0 | 9    |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_P\Data\BP011322\  
 Data File : BP008789.D  
 Acq On : 13 Jan 2022 14:37  
 Operator : CG/JU  
 Sample : N1098-03  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_P  
 ClientSampleId :  
 14-G-WATER

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_P\Methods\8270E-BP010622.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| Butane, 2-metho... | 3.064  | 112.2   | ng    | 9893180  | 1                     | 7.863  | 1763570 | 20.0 |
| Ethanol, 2-(2-b... | 10.457 | 3.4     | ng    | 388186   | 2                     | 10.669 | 2274380 | 20.0 |
| Safrole            | 12.134 | 2.7     | ng    | 304779   | 2                     | 10.669 | 2274380 | 20.0 |
| n-Hexadecanoic ... | 18.151 | 3.5     | ng    | 564871   | 4                     | 17.257 | 3226700 | 20.0 |
| Triphenylphosph... | 19.922 | 4.9     | ng    | 815451   | 5                     | 21.345 | 3353400 | 20.0 |
| 1-Heneicosanol     | 21.057 | 5.6     | ng    | 933727   | 5                     | 21.345 | 3353400 | 20.0 |
| unknown21.469      | 21.469 | 169.7   | ng    | 28452100 | 5                     | 21.345 | 3353400 | 20.0 |