

Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061022\  
 Data File : BG053878.D  
 Acq On : 10 Jun 2022 16:58  
 Operator : CG/JU  
 Sample : N3266-01  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 OH-WATER-0608

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\_G\Methods\8270-BG060222.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BG053878.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         | 5.520       | 356           | 363         | 376          | rBV3     | 39203          | 98021         | 5.16%           | 1.324%        |
| 2         | 5.655       | 380           | 386         | 395          | rVB      | 144122         | 248668        | 13.09%          | 3.360%        |
| 3         | 7.242       | 649           | 656         | 667          | rVB      | 89882          | 165571        | 8.71%           | 2.237%        |
| 4         | 8.088       | 794           | 800         | 808          | rVB      | 65426          | 114512        | 6.03%           | 1.547%        |
| 5         | 9.245       | 989           | 997         | 1006         | rBV      | 231162         | 433253        | 22.80%          | 5.853%        |
| 6         | 10.896      | 1271          | 1278        | 1286         | rBV      | 91333          | 172487        | 9.08%           | 2.330%        |
| 7         | 11.543      | 1381          | 1388        | 1394         | rBV2     | 16969          | 31937         | 1.68%           | 0.431%        |
| 8         | 13.341      | 1686          | 1694        | 1703         | rBV      | 716587         | 1194117       | 62.85%          | 16.133%       |
| 9         | 13.611      | 1732          | 1740        | 1746         | rBV      | 112484         | 188744        | 9.93%           | 2.550%        |
| 10        | 14.710      | 1918          | 1927        | 1934         | rBV      | 181437         | 304235        | 16.01%          | 4.110%        |
| 11        | 16.196      | 2173          | 2180        | 2194         | rBV      | 682326         | 1101566       | 57.98%          | 14.882%       |
| 12        | 17.453      | 2388          | 2394        | 2404         | rVB      | 254112         | 393348        | 20.70%          | 5.314%        |
| 13        | 18.346      | 2541          | 2546        | 2557         | rBV7     | 24702          | 59495         | 3.13%           | 0.804%        |
| 14        | 19.616      | 2758          | 2762        | 2768         | rBV7     | 12630          | 23856         | 1.26%           | 0.322%        |
| 15        | 20.062      | 2832          | 2838        | 2844         | rBV      | 1395723        | 1900013       | 100.00%         | 25.670%       |
| 16        | 21.372      | 3056          | 3061        | 3071         | rBV3     | 26680          | 49002         | 2.58%           | 0.662%        |
| 17        | 21.731      | 3115          | 3122        | 3130         | rBV2     | 267761         | 458261        | 24.12%          | 6.191%        |
| 18        | 24.998      | 3667          | 3678        | 3688         | rBV2     | 154912         | 464716        | 24.46%          | 6.278%        |

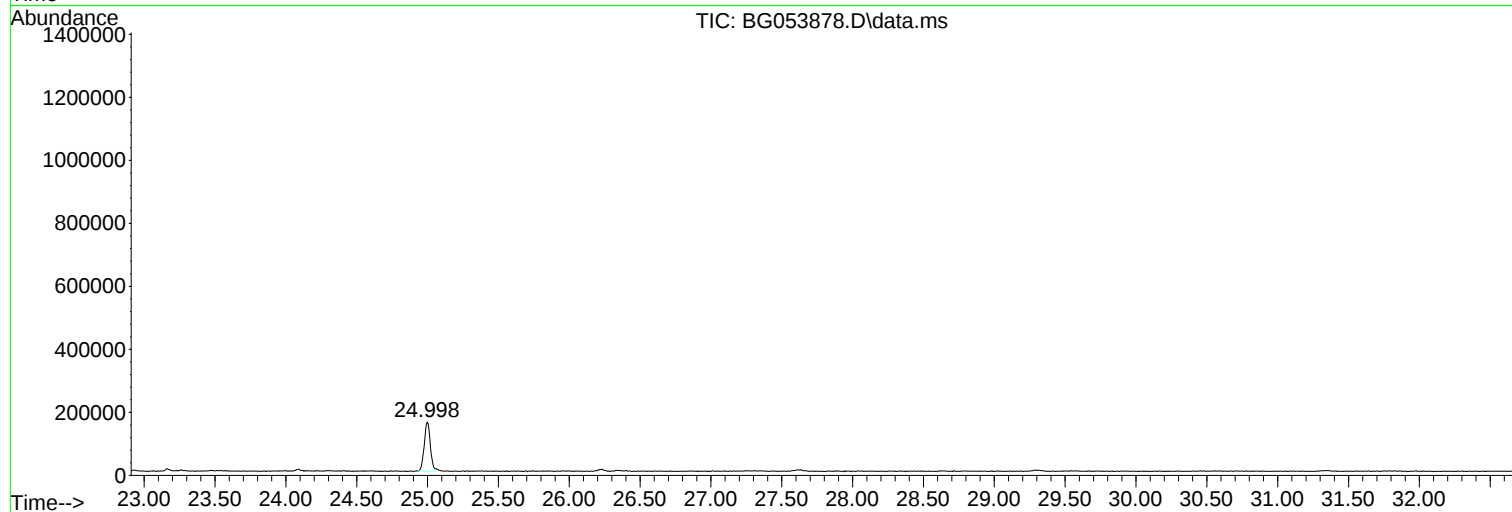
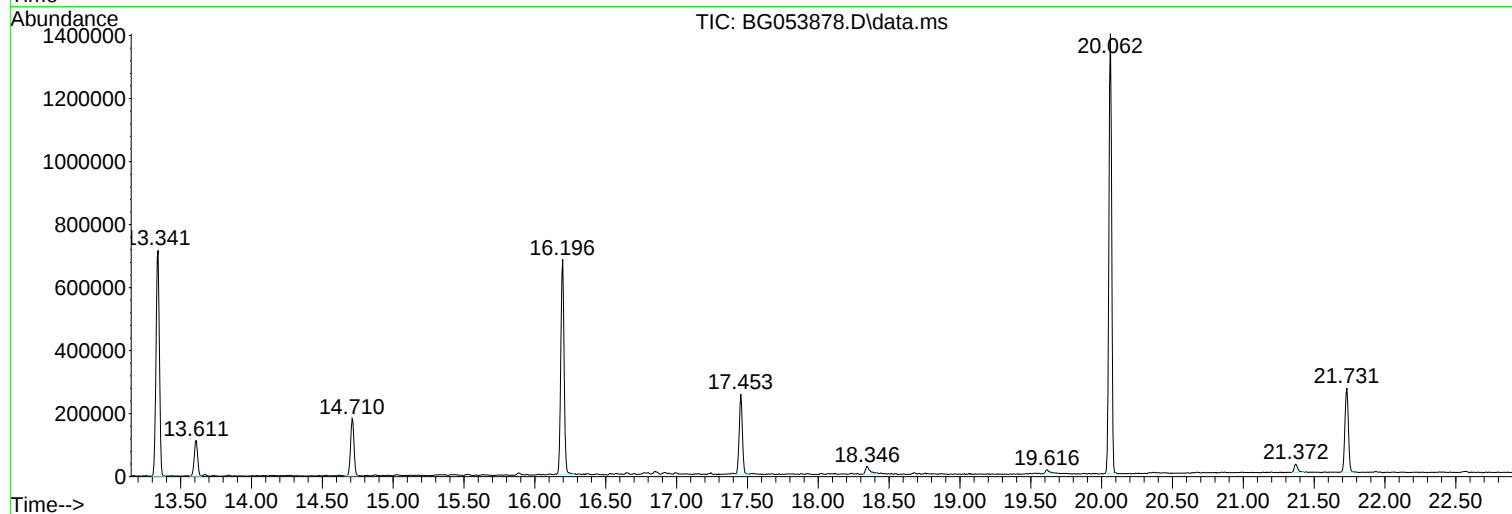
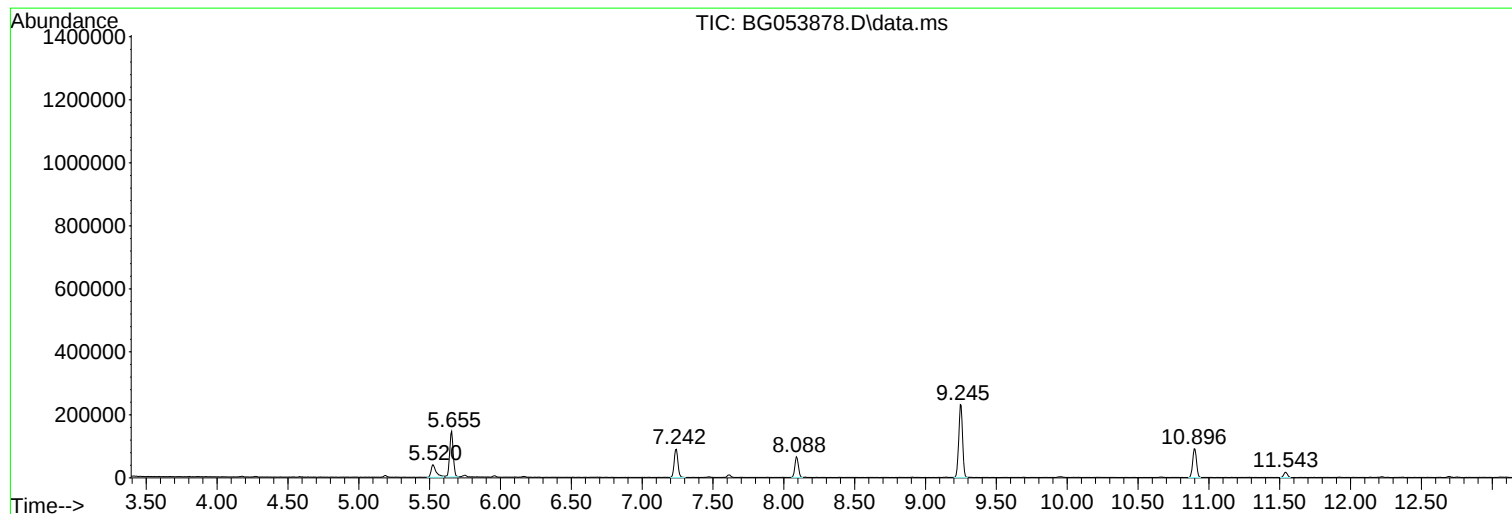
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BNA\_G  
ClientSampleId :  
OH-WATER-0608

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG060222.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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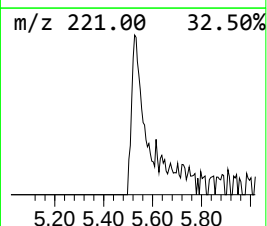
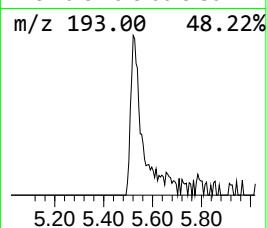
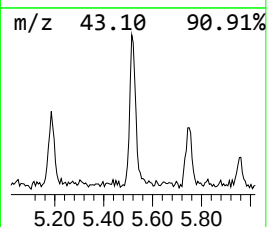
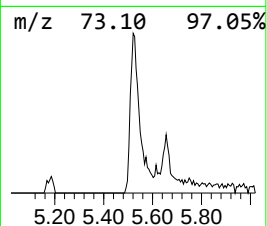
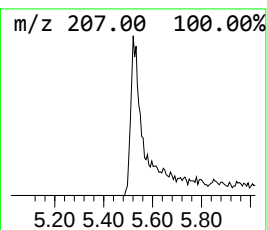
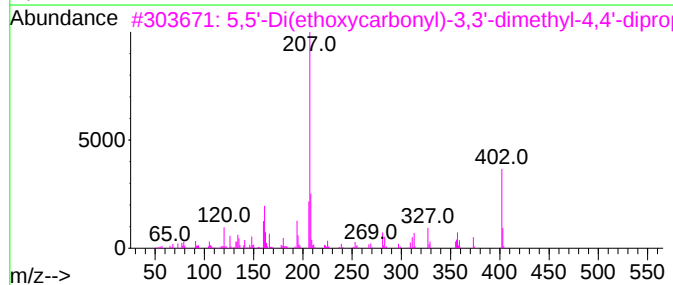
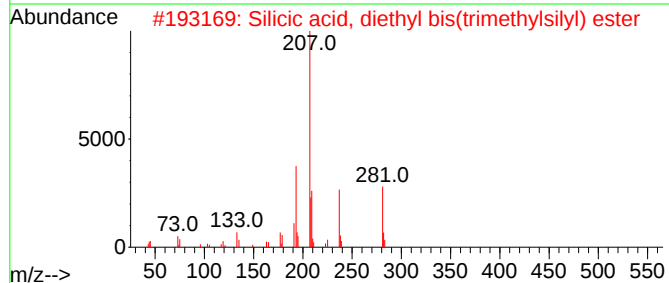
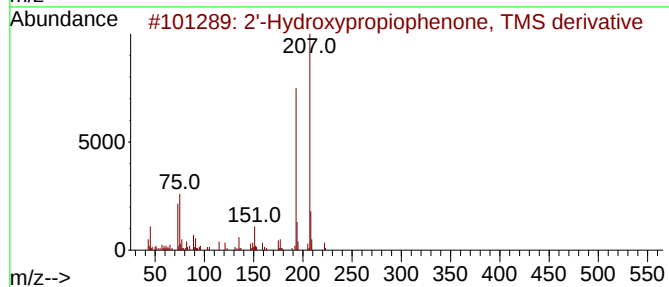
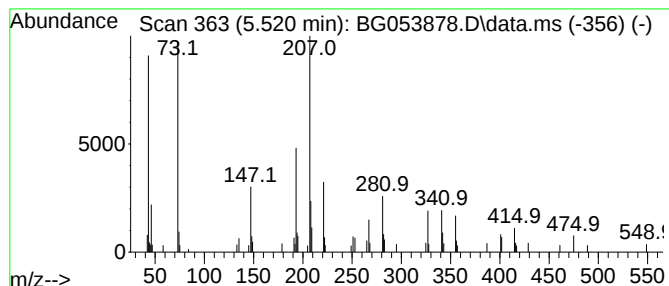
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown5.520 Concentration Rank 1

| R.T.  | EstConc  | Area  | Relative to ISTD       | R.T.  |
|-------|----------|-------|------------------------|-------|
| 5.520 | 17.12 ng | 98021 | 1,4-Dichlorobenzene-d4 | 8.088 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 2'-Hydroxypropiophenone, TMS der... | 222 | C12H18O2Si   | 033342-87-9  | 43      |      |      |
| 2    | Silicic acid, diethyl bis(trimet... | 296 | C10H28O4Si3  | 003555-45-1  | 40      |      |      |
| 3    | 5,5'-Di(ethoxycarbonyl)-3,3'-dim... | 402 | C23H34N2O4   | 102586-97-0  | 37      |      |      |
| 4    | 6-Fluoroindole, TMS derivative      | 207 | C11H14FNSi   | 1000468-35-0 | 35      |      |      |
| 5    | Octasiloxane, 1,1,3,3,5,5,7,7,9,... | 578 | C16H50O7Si8  | 019095-24-0  | 32      |      |      |



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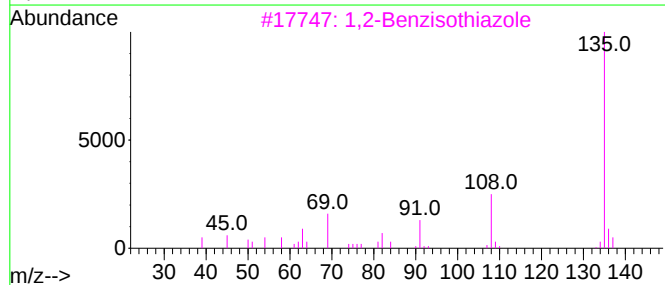
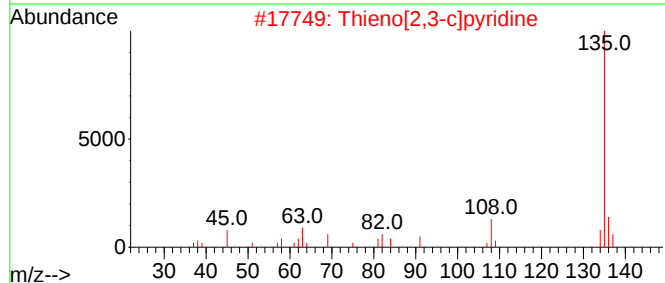
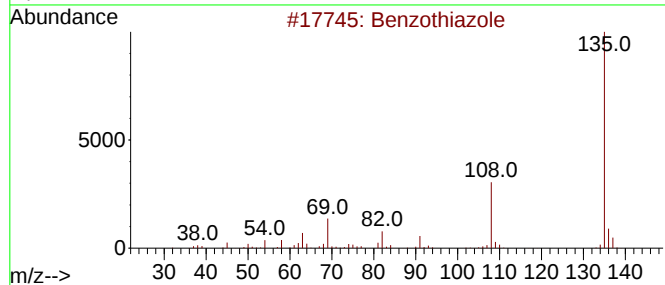
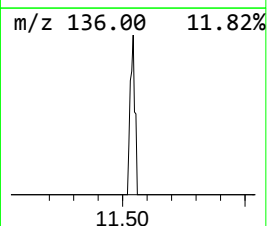
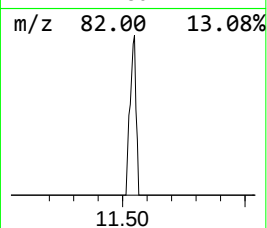
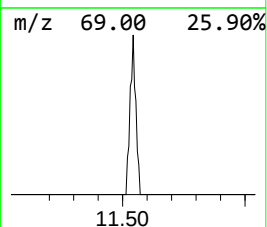
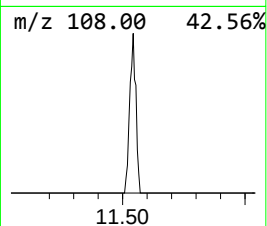
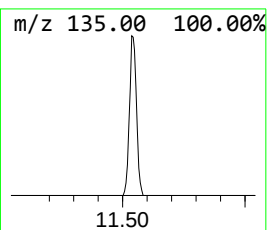
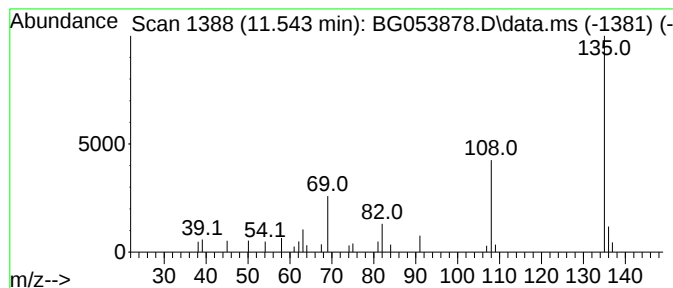
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG060222.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Benzothiazole Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 11.543 | 3.70 ng | 31937 | Naphthalene-d8   | 10.896 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Benzothiazole                       | 135 | C7H5NS  | 000095-16-9 | 95   |
| 2    |    |   | Thieno[2,3-c]pyridine               | 135 | C7H5NS  | 000272-12-8 | 81   |
| 3    |    |   | 1,2-Benzisothiazole                 | 135 | C7H5NS  | 000272-16-2 | 80   |
| 4    |    |   | Adenine                             | 135 | C5H5N5  | 000073-24-5 | 64   |
| 5    |    |   | 1H-Pyrazolo[3,4-d]pyrimidin-4-amine | 135 | C5H5N5  | 002380-63-4 | 64   |



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ALS Vial : 8 Sample Multiplier: 1

Instrument :  
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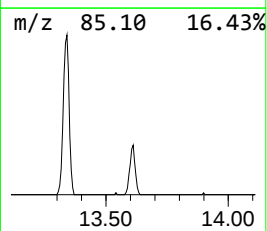
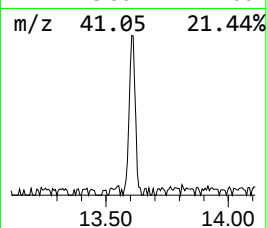
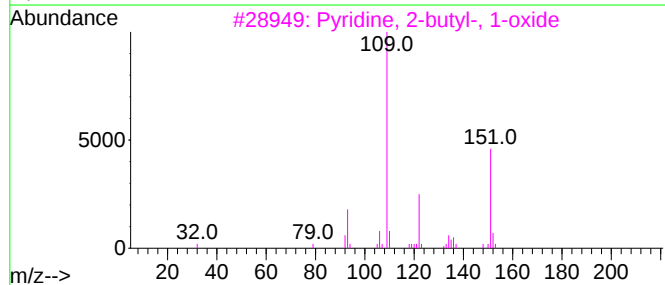
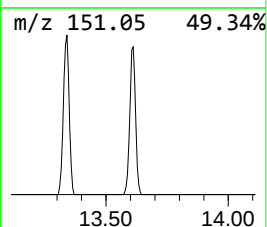
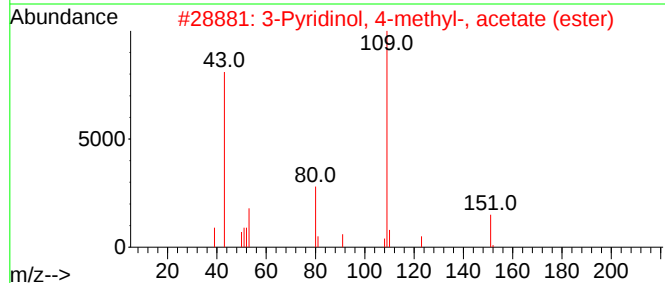
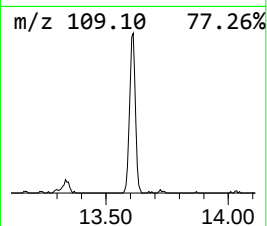
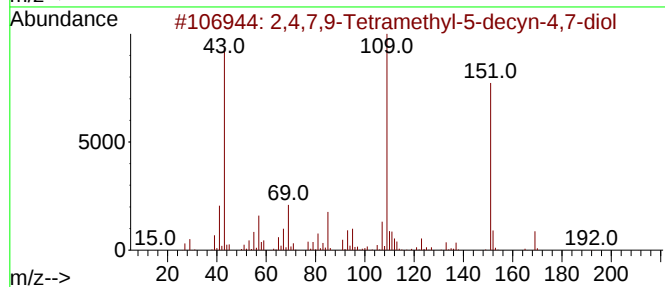
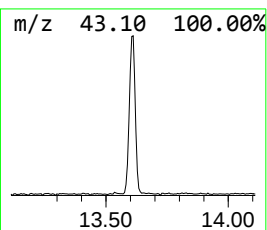
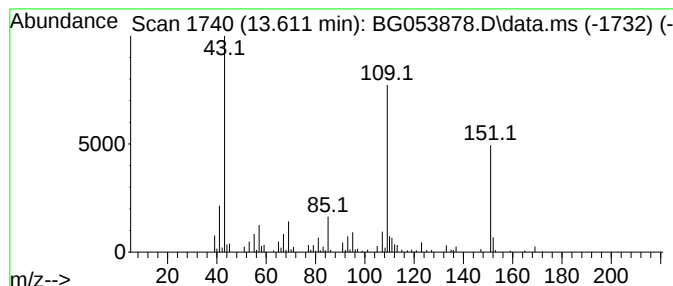
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TIC Integration Parameters: LSCINT.P

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Peak Number 3 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD |          | R.T.         |      |
|-----------|-------------------------------------|--------|------------------|----------|--------------|------|
| 13.611    | 12.41 ng                            | 188744 | Acenaphthene-d10 |          | 14.710       |      |
| Hit# of 5 | Tentative ID                        |        | MW               | MolForm  | CAS#         | Qual |
| 1         | 2,4,7,9-Tetramethyl-5-decyn-4,7-... |        | 226              | C14H26O2 | 000126-86-3  | 91   |
| 2         | 3-Pyridinol, 4-methyl-, acetate ... |        | 151              | C8H9NO2  | 001006-96-8  | 59   |
| 3         | Pyridine, 2-butyl-, 1-oxide         |        | 151              | C9H13NO  | 031396-32-4  | 59   |
| 4         | Metacetamol                         |        | 151              | C8H9NO2  | 000621-42-1  | 59   |
| 5         | N-Cyclopropyl-p-fluorobenzylamine   |        | 165              | C10H12FN | 1000250-88-9 | 47   |



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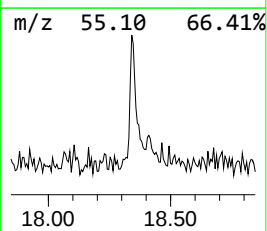
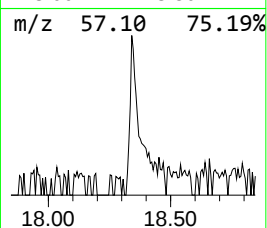
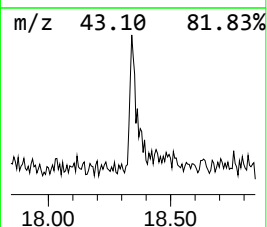
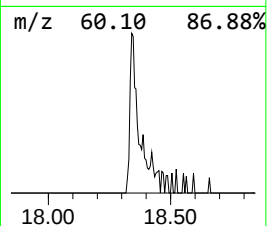
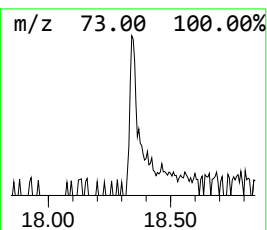
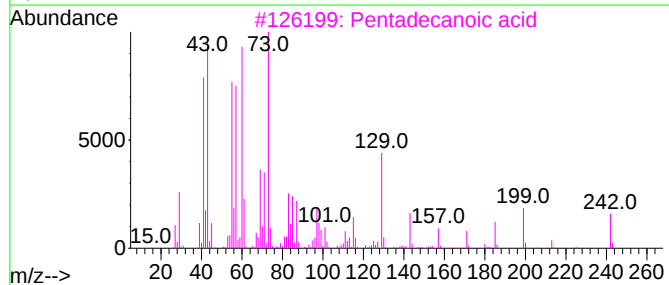
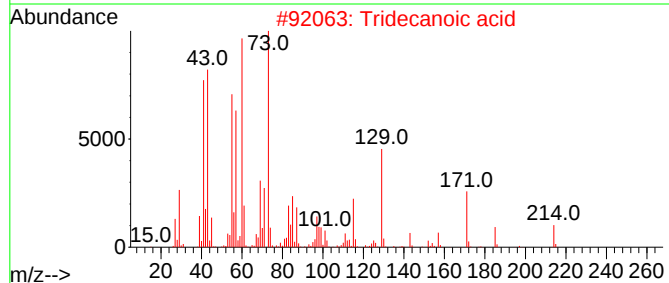
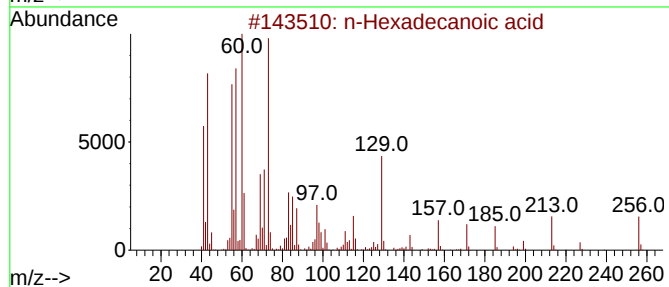
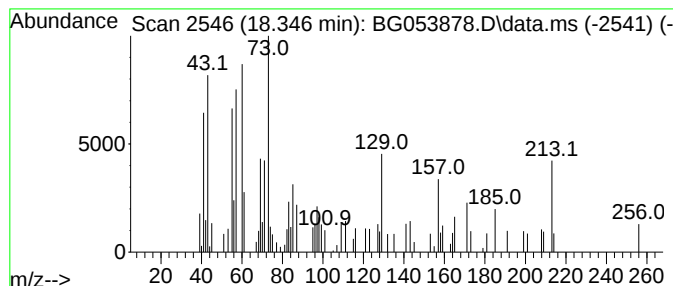
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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\*\*\*\*\*  
Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 18.346 | 3.03 ng | 59495 | Phenanthrene-d10 | 17.453 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 83   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 64   |
| 4    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 50   |
| 5    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 47   |



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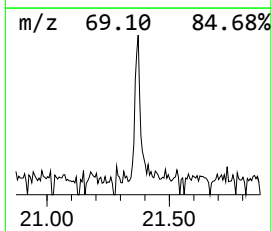
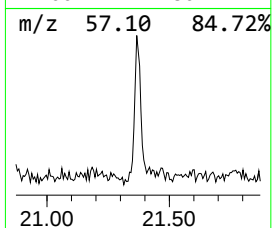
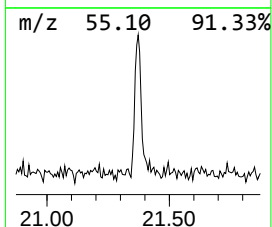
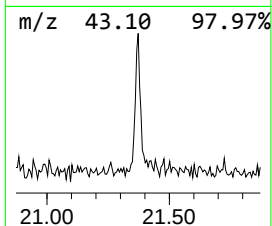
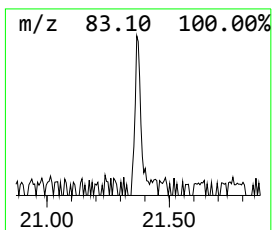
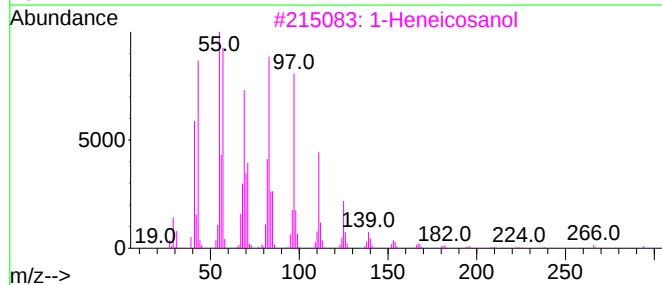
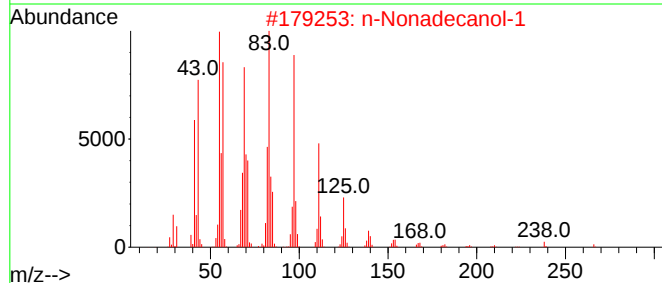
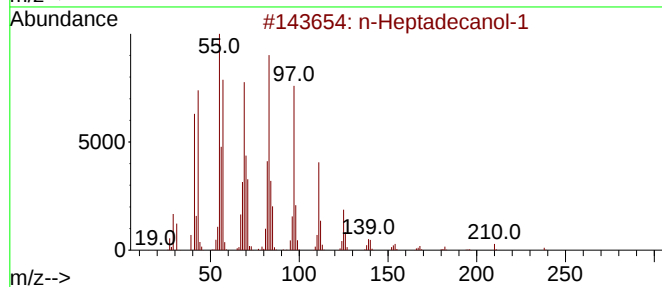
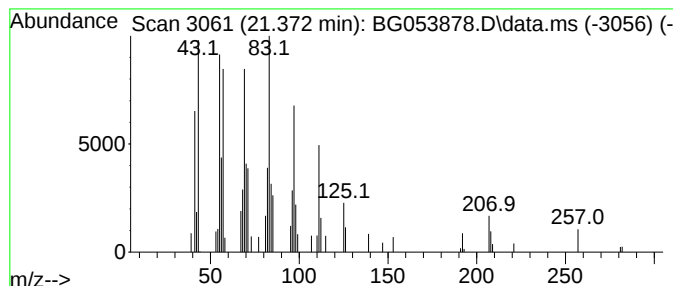
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\*\*\*\*\*  
Peak Number 5 n-Heptadecanol-1 Concentration Rank 5

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 21.372 | 2.14 ng | 49002 | Chrysene-d12     | 21.731 |

| Hit# | of | 5 | Tentative ID                | MW  | MolForm    | CAS#        | Qual |
|------|----|---|-----------------------------|-----|------------|-------------|------|
| 1    |    |   | n-Heptadecanol-1            | 256 | C17H36O    | 001454-85-9 | 94   |
| 2    |    |   | n-Nonadecanol-1             | 284 | C19H40O    | 001454-84-8 | 94   |
| 3    |    |   | 1-Heneicosanol              | 312 | C21H44O    | 015594-90-8 | 94   |
| 4    |    |   | Tetradecyl trifluoroacetate | 310 | C16H29F3O2 | 006222-02-2 | 93   |
| 5    |    |   | 1-Octadecanol               | 270 | C18H38O    | 000112-92-5 | 93   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_G\Data\BG061022\  
Data File : BG053878.D  
Acq On : 10 Jun 2022 16:58  
Operator : CG/JU  
Sample : N3266-01  
Misc :  
ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
OH-WATER-0608

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_G\Methods\8270-BG060222.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 |
| unknown5.520       | 5.520  | 17.1    | ng    | 98021    | 1                     | 8.088  | 114512 | 20.0 |
| Benzothiazole      | 11.543 | 3.7     | ng    | 31937    | 2                     | 10.896 | 172487 | 20.0 |
| 2,4,7,9-Tetrame... | 13.611 | 12.4    | ng    | 188744   | 3                     | 14.710 | 304235 | 20.0 |
| n-Hexadecanoic ... | 18.346 | 3.0     | ng    | 59495    | 4                     | 17.453 | 393348 | 20.0 |
| n-Heptadecanol-1   | 21.372 | 2.1     | ng    | 49002    | 5                     | 21.731 | 458261 | 20.0 |