

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\  
 Data File : BM016677.D  
 Acq On : 05 Sep 2018 18:30  
 Operator : SJ/JU  
 Sample : J4741-21  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 A0C2-03-A

Integration Parameters: rteint.p  
 Integrator: RTE  
 Smoothing : ON  
 Sampling : 1  
 Start Thrs: 0.2  
 Stop Thrs : 0  
 Filtering: 5  
 Min Area: 3 % of largest Peak  
 Max Peaks: 100  
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >  
 Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM082118.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 5.516       | 374           | 379         | 392          | rBV      | 444767         | 830041        | 9.01%           | 2.500%        |
| 2         | 7.151       | 650           | 657         | 674          | rBV      | 266706         | 544516        | 5.91%           | 1.640%        |
| 3         | 7.492       | 709           | 715         | 730          | rBV      | 1200957        | 2023873       | 21.98%          | 6.095%        |
| 4         | 7.963       | 787           | 795         | 811          | rBV      | 301093         | 556744        | 6.05%           | 1.677%        |
| 5         | 8.281       | 841           | 849         | 865          | rBV      | 1312600        | 2221377       | 24.12%          | 6.690%        |
| 6         | 9.151       | 990           | 997         | 1013         | rBV      | 776394         | 1412299       | 15.34%          | 4.253%        |
| 7         | 10.769      | 1266          | 1272        | 1277         | rBV      | 348209         | 591825        | 6.43%           | 1.782%        |
| 8         | 10.822      | 1277          | 1281        | 1292         | rVB2     | 73840          | 164271        | 1.78%           | 0.495%        |
| 9         | 13.221      | 1679          | 1689        | 1701         | rBV      | 3205487        | 4414373       | 47.94%          | 13.295%       |
| 10        | 13.474      | 1724          | 1732        | 1741         | rVB2     | 133384         | 223024        | 2.42%           | 0.672%        |
| 11        | 14.068      | 1828          | 1833        | 1845         | rBV      | 232011         | 347030        | 3.77%           | 1.045%        |
| 12        | 14.610      | 1919          | 1925        | 1933         | rBV      | 501521         | 790453        | 8.58%           | 2.381%        |
| 13        | 16.104      | 2172          | 2179        | 2191         | rBV      | 3179022        | 4498287       | 48.85%          | 13.547%       |
| 14        | 17.351      | 2386          | 2391        | 2398         | rBV      | 724873         | 1111987       | 12.08%          | 3.349%        |
| 15        | 18.209      | 2532          | 2537        | 2544         | rBV2     | 213697         | 308017        | 3.34%           | 0.928%        |
| 16        | 19.474      | 2747          | 2752        | 2759         | rBV5     | 125176         | 199797        | 2.17%           | 0.602%        |
| 17        | 19.945      | 2826          | 2832        | 2839         | rBV      | 8288814        | 9208336       | 100.00%         | 27.732%       |
| 18        | 21.503      | 3092          | 3097        | 3103         | rBV      | 1270861        | 1631536       | 17.72%          | 4.914%        |
| 19        | 22.615      | 3283          | 3286        | 3291         | rVB      | 249237         | 311249        | 3.38%           | 0.937%        |
| 20        | 23.768      | 3476          | 3482        | 3489         | rVB      | 934176         | 1815237       | 19.71%          | 5.467%        |

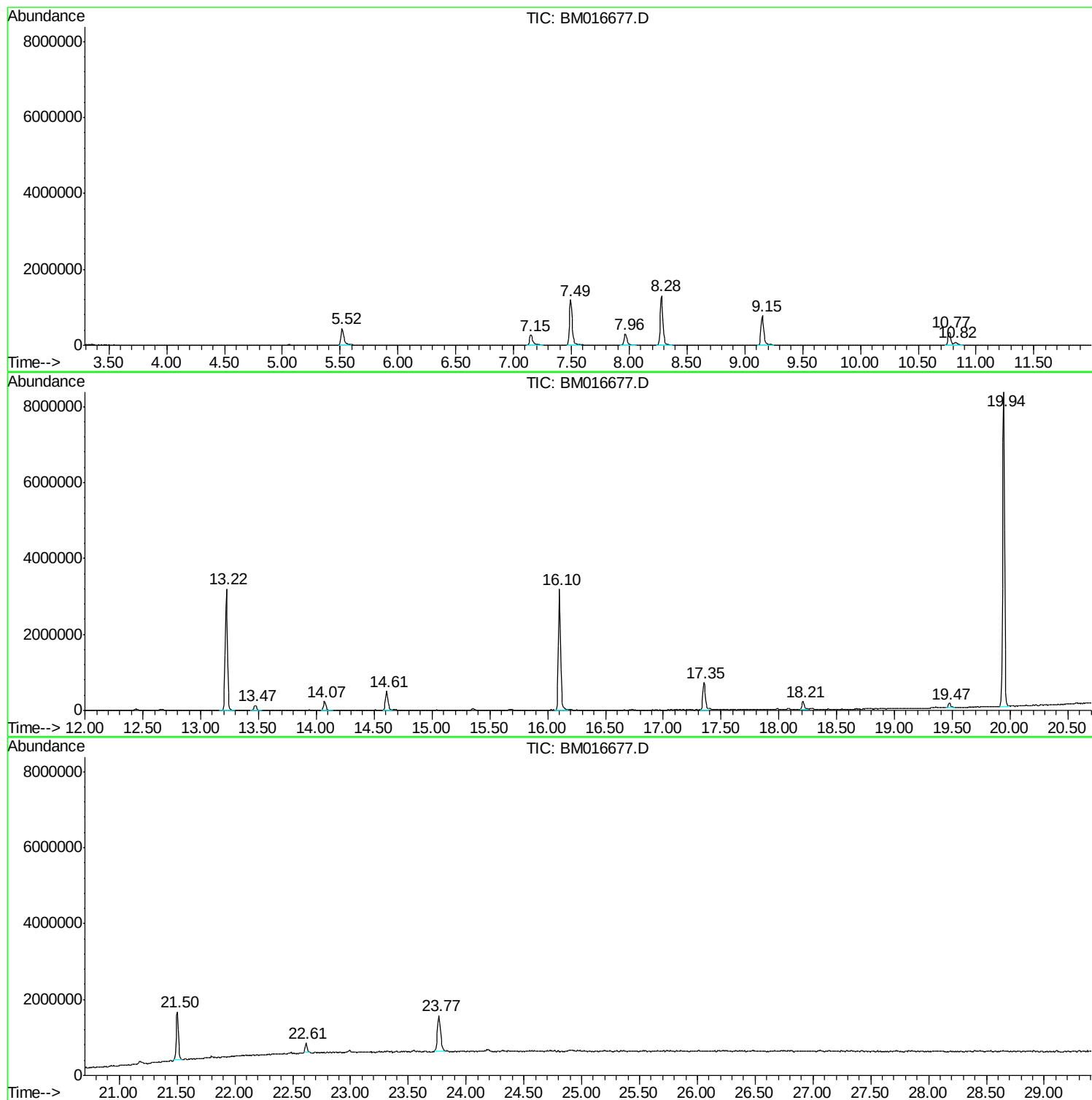
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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090518\  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

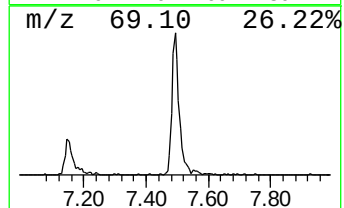
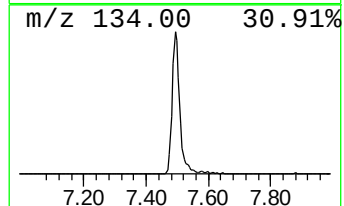
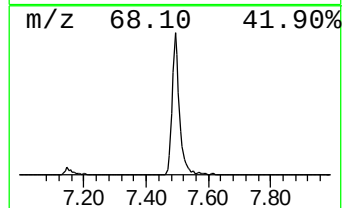
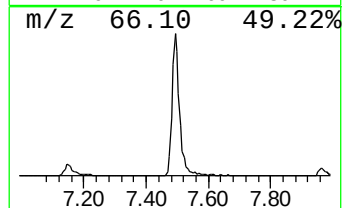
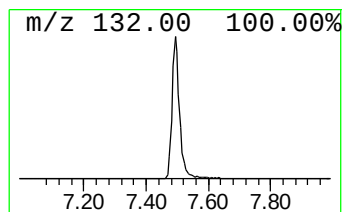
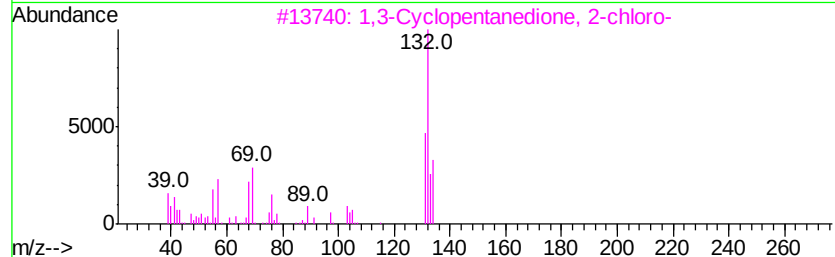
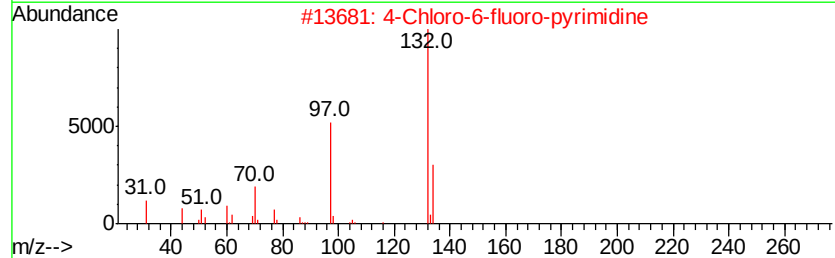
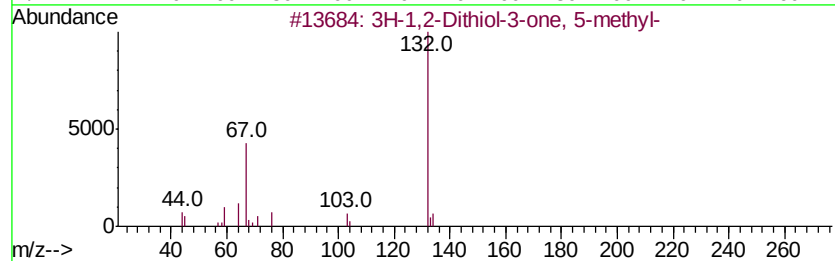
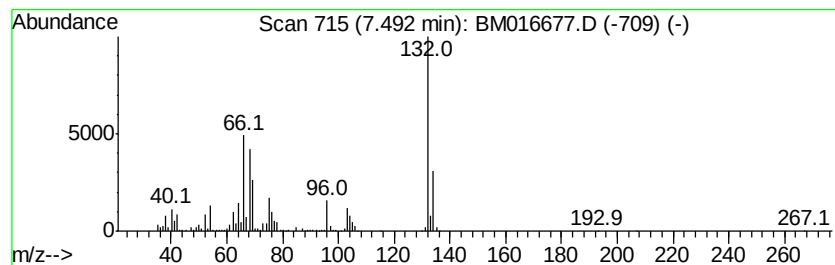
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown7.49 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.49 | 72.70 ng | 2023870 | 1,4-Dichlorobenzene-d4 | 7.97 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 3H-1,2-Dithiol-3-one, 5-methyl-     | 132 | C4H4OS2   | 003620-08-4 | 14   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6 | 12   |
| 3    |    | 1,3-Cyclopentanedione, 2-chloro-    | 132 | C5H5ClO2  | 014203-19-1 | 10   |
| 4    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5 | 10   |
| 5    |    | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6 | 10   |



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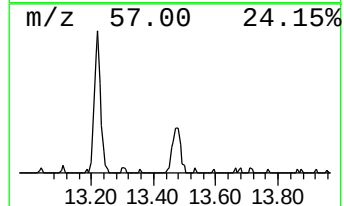
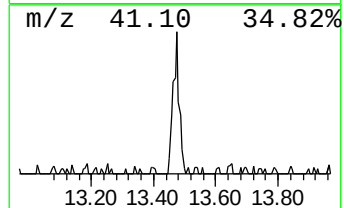
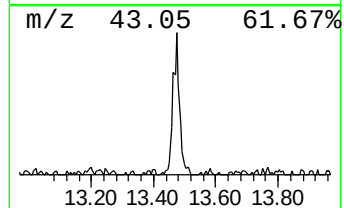
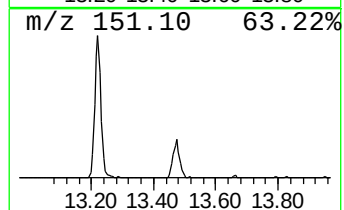
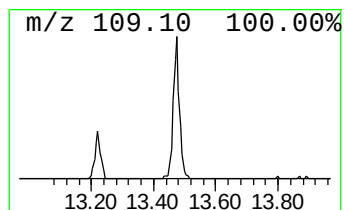
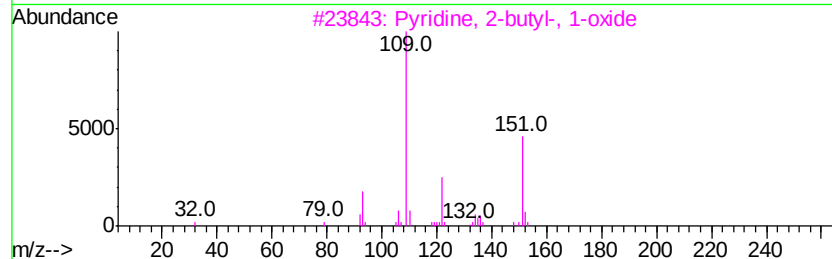
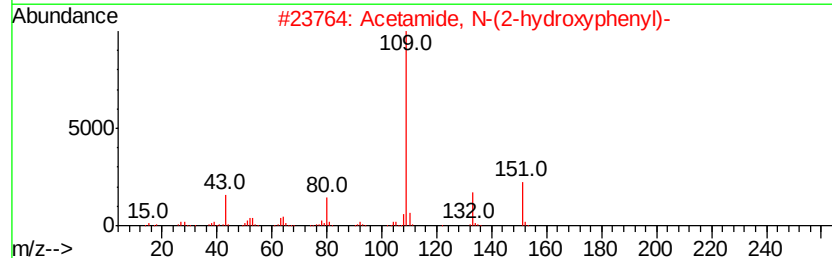
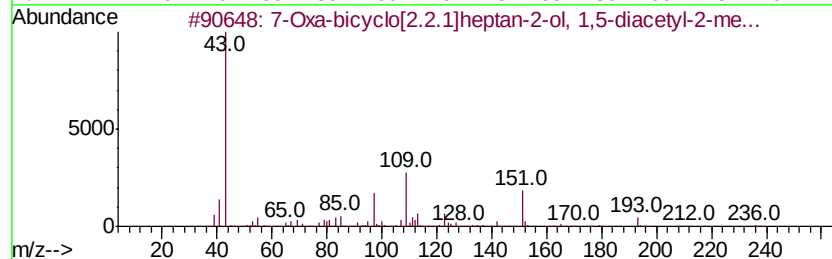
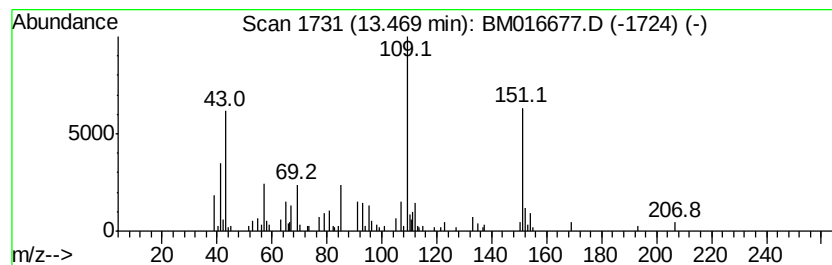
Instrument :  
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ClientSampleId :  
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 7-Oxa-bicyclo[2.2.1]heptan-... Concentration Rank 3

| R.T.      | EstConc                              | Area   | Relative to ISTD | R.T.        |      |
|-----------|--------------------------------------|--------|------------------|-------------|------|
| 13.47     | 5.64 ng                              | 223024 | Acenaphthene-d10 | 14.60       |      |
| Hit# of 5 | Tentative ID                         | MW     | MolForm          | CAS#        | Qual |
| 1         | 7-Oxa-bicyclo[2.2.1]heptan-2-ol, ... | 254    | C14H22O4         | 329362-13-2 | 72   |
| 2         | Acetamide, N-(2-hydroxyphenyl)-      | 151    | C8H9NO2          | 000614-80-2 | 52   |
| 3         | Pyridine, 2-butyl-, 1-oxide          | 151    | C9H13NO          | 031396-32-4 | 52   |
| 4         | m-Isopropoxyaniline                  | 151    | C9H13NO          | 041406-00-2 | 50   |
| 5         | 3-Pyridinol, 4-methyl-, acetate ...  | 151    | C8H9NO2          | 001006-96-8 | 50   |



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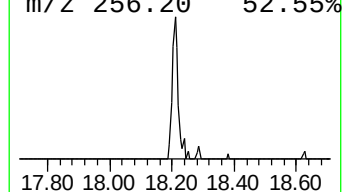
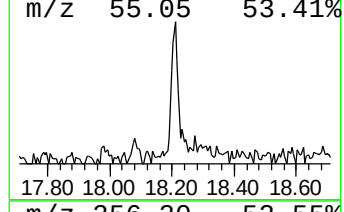
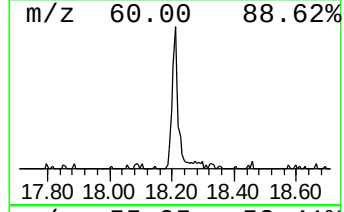
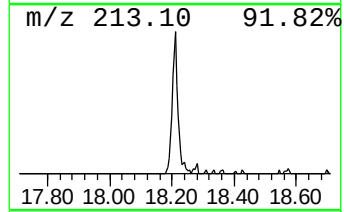
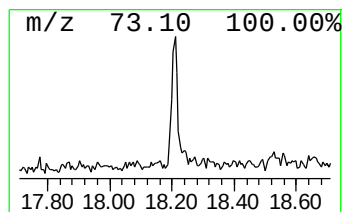
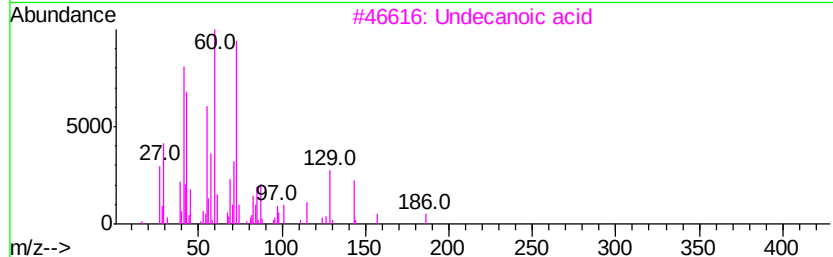
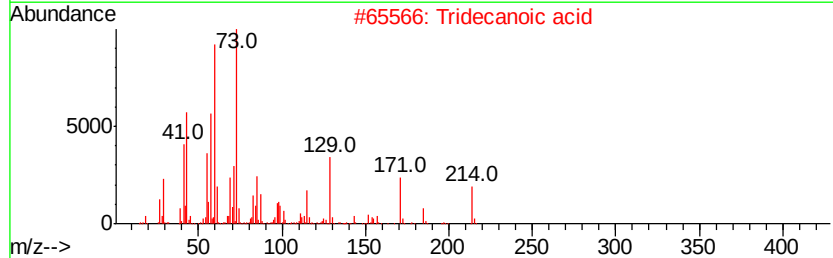
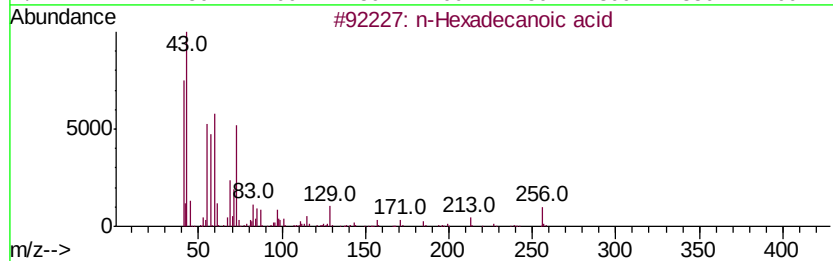
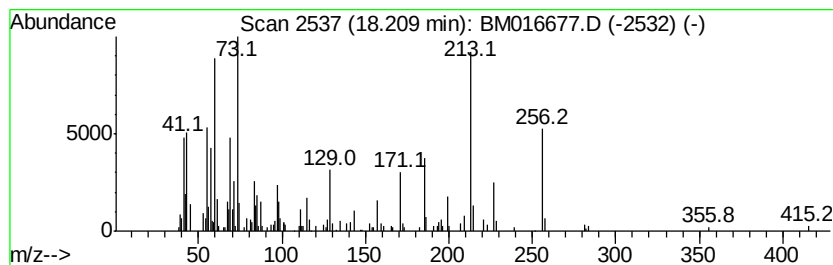
Instrument :  
BNA\_M  
ClientSampleId :  
A0C2-03-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.      | EstConc             | Area   | Relative to ISTD | R.T.        |      |
|-----------|---------------------|--------|------------------|-------------|------|
| 18.21     | 5.54 ng             | 308017 | Phenanthrene-d10 | 17.35       |      |
| Hit# of 5 | Tentative ID        | MW     | MolForm          | CAS#        | Qual |
| 1         | n-Hexadecanoic acid | 256    | C16H32O2         | 000057-10-3 | 95   |
| 2         | Tridecanoic acid    | 214    | C13H26O2         | 000638-53-9 | 94   |
| 3         | Undecanoic acid     | 186    | C11H22O2         | 000112-37-8 | 55   |
| 4         | Lumiflavine         | 256    | C13H12N4O2       | 001088-56-8 | 41   |
| 5         | n-Decanoic acid     | 172    | C10H20O2         | 000334-48-5 | 35   |



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ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
A0C2-03-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

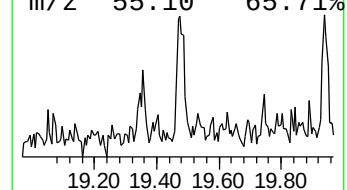
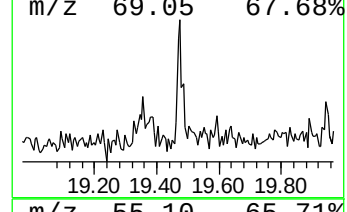
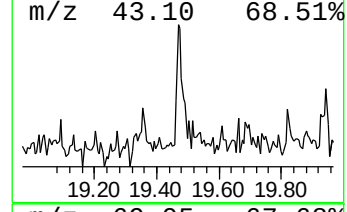
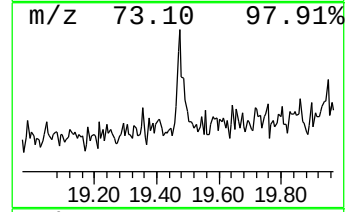
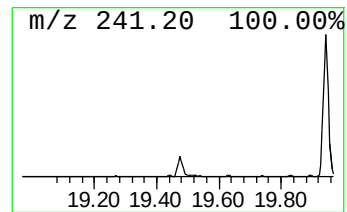
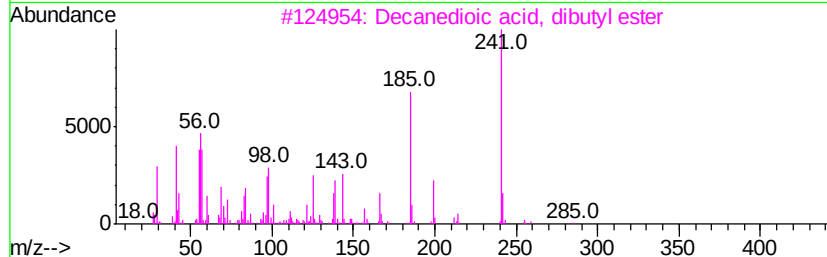
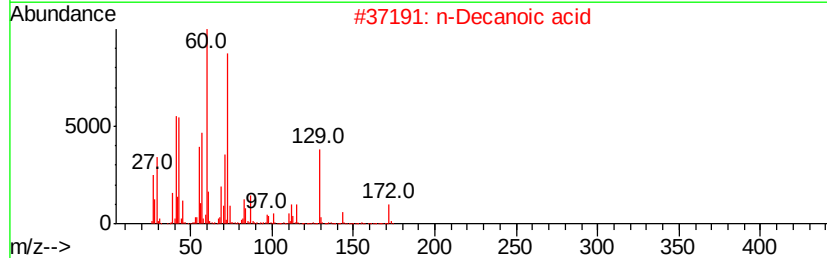
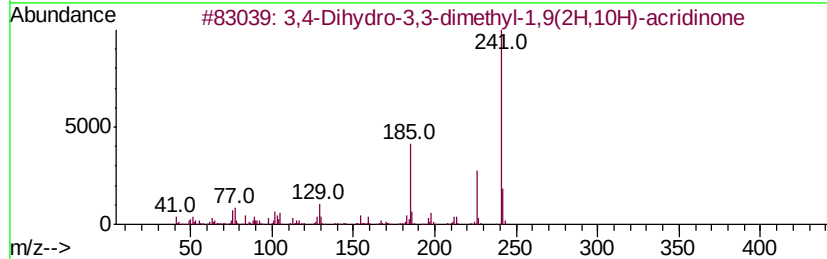
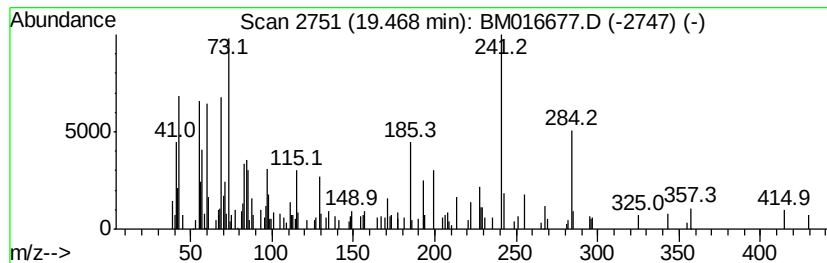
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown19.47 Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 19.47 | 2.45 ng | 199797 | Chrysene-d12     | 21.50 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 3,4-Dihydro-3,3-dimethyl-1,9(2H,... | 241 | C15H15N02    | 1000212-95-2 | 35      |      |      |
| 2    | n-Decanoic acid                     | 172 | C10H20O2     | 000334-48-5  | 35      |      |      |
| 3    | Decanedioic acid, dibutyl ester     | 314 | C18H34O4     | 000109-43-3  | 35      |      |      |
| 4    | Tetradecanoic acid                  | 228 | C14H28O2     | 000544-63-8  | 22      |      |      |
| 5    | 8-Nitro-1,2-dimethylpyrrolo[3,2-... | 241 | C13H11N3O2   | 072793-29-4  | 18      |      |      |



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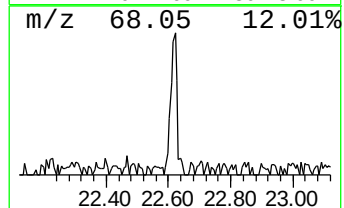
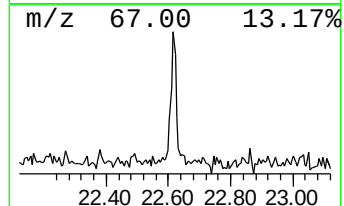
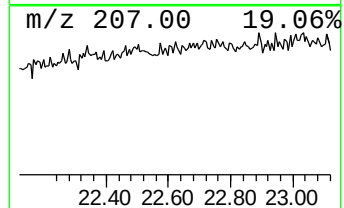
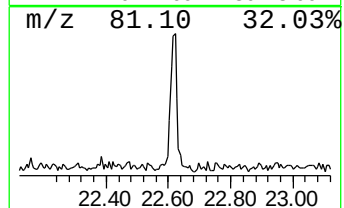
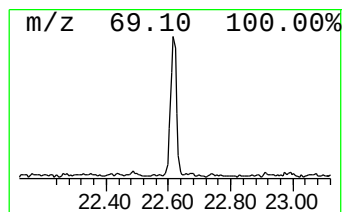
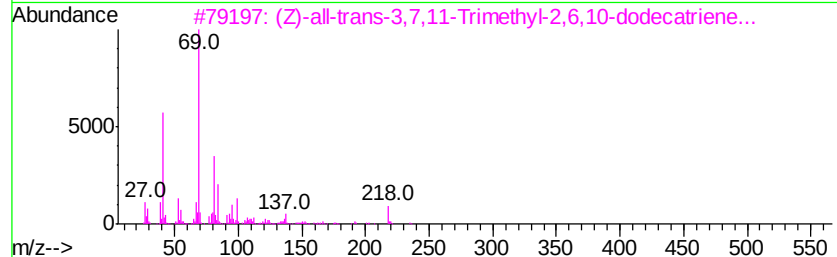
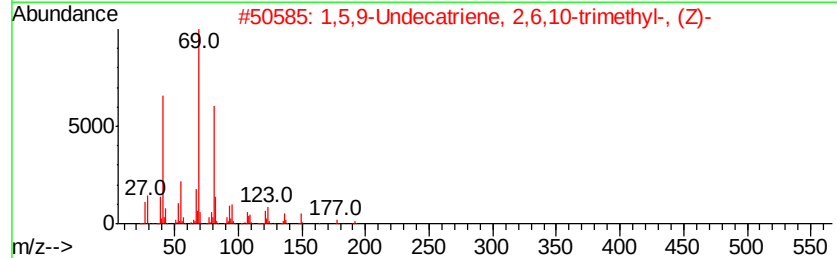
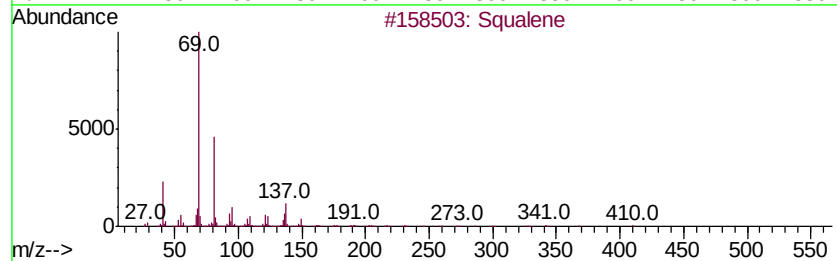
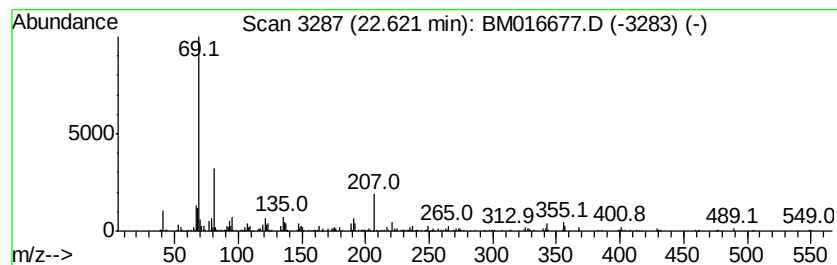
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TIC Integration Parameters: LSCINT.P

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Peak Number 6 Squalene Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 22.62 | 3.82 ng | 311249 | Chrysene-d12     | 21.50 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Squalene                            | 410 | C30H50   | 007683-64-9  | 81   |
| 2    |    | 1,5,9-Undecatriene, 2,6,10-trime... | 192 | C14H24   | 062951-96-6  | 74   |
| 3    |    | (Z)-all-trans-3,7,11-Trimethyl-2... | 235 | C15H25NO | 123257-83-0  | 74   |
| 4    |    | 2,6,10-Dodecatrien-1-ol, 3,7,11-... | 222 | C15H26O  | 000106-28-5  | 72   |
| 5    |    | (E)-all-trans-3,7,11-Trimethyl-2... | 235 | C15H25NO | 1000161-30-7 | 64   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_M\DATA\BM090518\  
Data File : BM016677.D  
Acq On : 05 Sep 2018 18:30  
Operator : SJ/JU  
Sample : J4741-21  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
A0C2-03-A

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM082118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| unknown7.49          | 7.49  | 72.7    | ng    | 2023870  | 1                     | 7.97  | 556744  | 20.0 |
| 7-Oxa-bicyclo[2.2... | 13.47 | 5.6     | ng    | 223024   | 3                     | 14.60 | 790453  | 20.0 |
| n-Hexadecanoic acid  | 18.21 | 5.5     | ng    | 308017   | 4                     | 17.35 | 1111990 | 20.0 |
| unknown19.47         | 19.47 | 2.5     | ng    | 199797   | 5                     | 21.50 | 1631540 | 20.0 |
| Squalene             | 22.62 | 3.8     | ng    | 311249   | 5                     | 21.50 | 1631540 | 20.0 |