

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG031819\  
 Data File : BG039988.D  
 Acq On : 19 Mar 2019 3:09  
 Operator : JU/SJ  
 Sample : K1930-01  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_G  
 ClientSampleId :  
 TP-3

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\_G\METHODS\8270-BG030419.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         | 3.196       | 13            | 18          | 27           | rBV      | 92188          | 181172        | 7.36%           | 1.116%        |
| 2         | 3.272       | 27            | 31          | 42           | rVB      | 131488         | 195259        | 7.93%           | 1.203%        |
| 3         | 5.693       | 435           | 443         | 453          | rVB      | 777996         | 1215971       | 49.41%          | 7.492%        |
| 4         | 7.296       | 706           | 716         | 731          | rBV      | 828994         | 1506924       | 61.23%          | 9.285%        |
| 5         | 7.672       | 773           | 780         | 791          | rVB      | 748480         | 1302152       | 52.91%          | 8.023%        |
| 6         | 8.142       | 853           | 860         | 872          | rVB      | 148775         | 257616        | 10.47%          | 1.587%        |
| 7         | 8.471       | 908           | 916         | 925          | rVB      | 501739         | 889873        | 36.16%          | 5.483%        |
| 8         | 9.323       | 1051          | 1061        | 1070         | rBV      | 480577         | 855585        | 34.76%          | 5.272%        |
| 9         | 10.968      | 1332          | 1341        | 1348         | rBV      | 208443         | 379405        | 15.42%          | 2.338%        |
| 10        | 13.394      | 1747          | 1754        | 1761         | rVB      | 1153414        | 1742924       | 70.82%          | 10.739%       |
| 11        | 14.216      | 1888          | 1894        | 1899         | rBV      | 87616          | 127675        | 5.19%           | 0.787%        |
| 12        | 14.768      | 1982          | 1988        | 1997         | rVB2     | 358300         | 574420        | 23.34%          | 3.539%        |
| 13        | 16.261      | 2234          | 2242        | 2254         | rBV      | 1070406        | 1624497       | 66.01%          | 10.010%       |
| 14        | 17.518      | 2449          | 2456        | 2467         | rVB      | 492906         | 747372        | 30.37%          | 4.605%        |
| 15        | 18.364      | 2595          | 2600        | 2606         | rBV3     | 33053          | 51817         | 2.11%           | 0.319%        |
| 16        | 20.108      | 2891          | 2897        | 2903         | rBV      | 1885002        | 2461122       | 100.00%         | 15.164%       |
| 17        | 21.389      | 3110          | 3115        | 3125         | rBV2     | 62936          | 128548        | 5.22%           | 0.792%        |
| 18        | 21.800      | 3177          | 3185        | 3192         | rBV2     | 473521         | 819123        | 33.28%          | 5.047%        |
| 19        | 21.941      | 3205          | 3209        | 3214         | rVB2     | 23655          | 35518         | 1.44%           | 0.219%        |
| 20        | 22.564      | 3311          | 3315        | 3320         | rVV3     | 29278          | 42587         | 1.73%           | 0.262%        |
| 21        | 22.634      | 3323          | 3327        | 3337         | rVB3     | 15049          | 32765         | 1.33%           | 0.202%        |
| 22        | 23.281      | 3432          | 3437        | 3444         | rVB3     | 34137          | 60215         | 2.45%           | 0.371%        |
| 23        | 24.115      | 3573          | 3579        | 3586         | rVB3     | 38669          | 85524         | 3.48%           | 0.527%        |
| 24        | 25.102      | 3739          | 3747        | 3748         | rBV2     | 30227          | 61214         | 2.49%           | 0.377%        |
| 25        | 25.160      | 3749          | 3757        | 3770         | rVB      | 261120         | 766644        | 31.15%          | 4.724%        |
| 26        | 26.271      | 3939          | 3946        | 3956         | rVB4     | 28430          | 83615         | 3.40%           | 0.515%        |

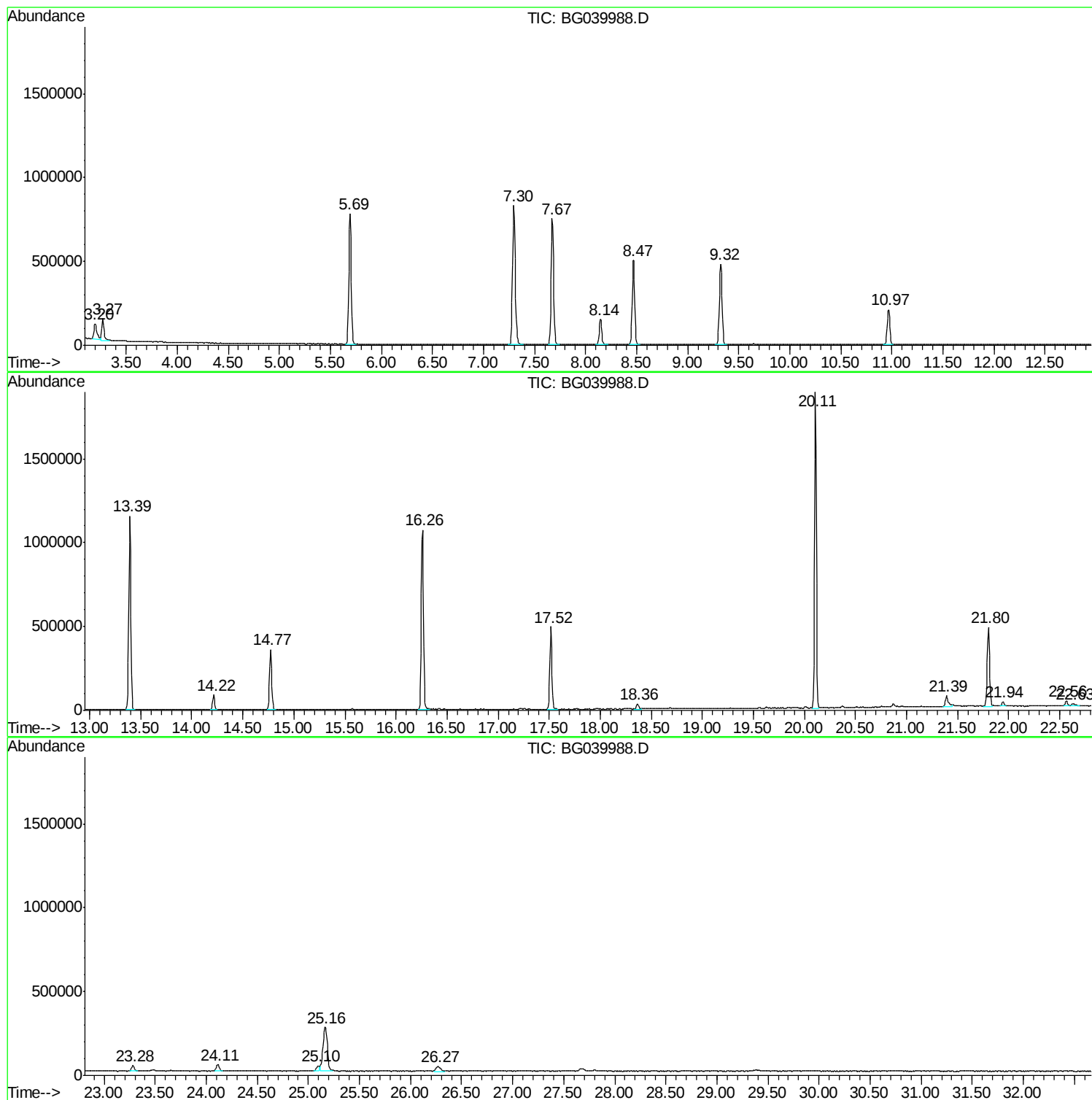
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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P



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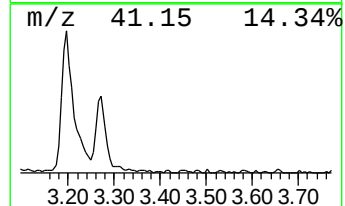
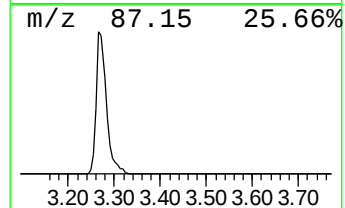
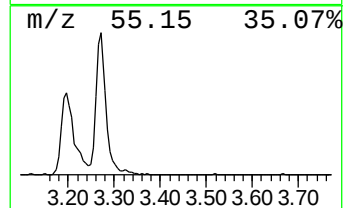
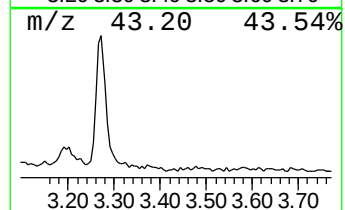
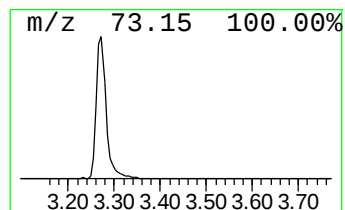
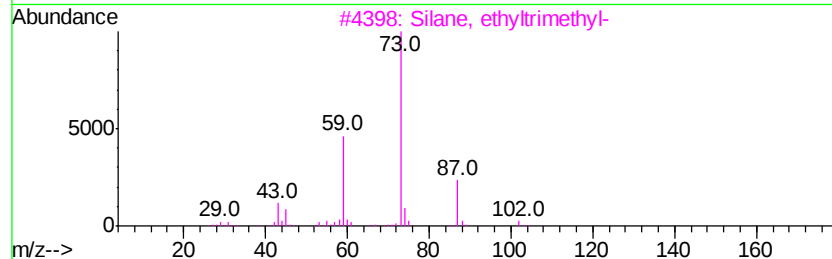
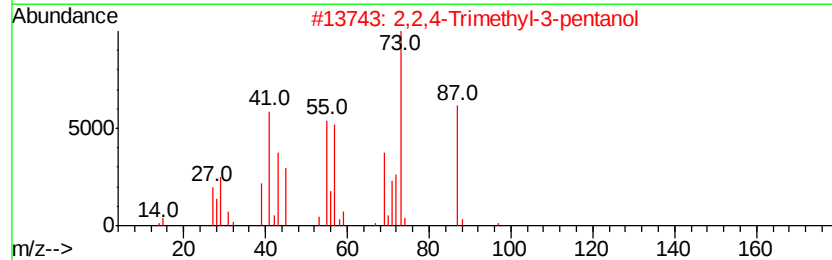
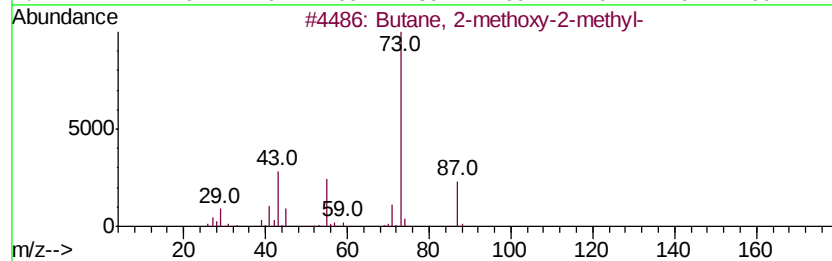
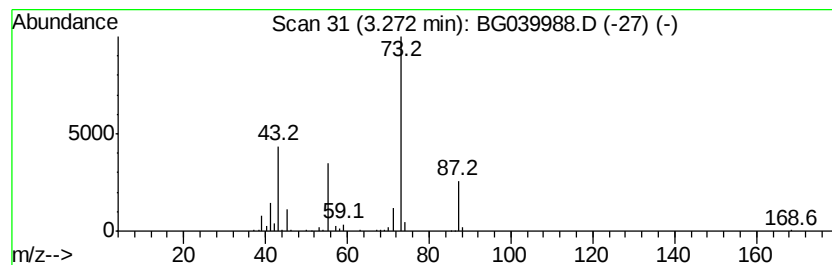
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 3.27 | 15.16 ng | 195259 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID                   | MW  | MolForm | CAS#        | Qual |
|------|----|--------------------------------|-----|---------|-------------|------|
| 1    | 5  | Butane, 2-methoxy-2-methyl-    | 102 | C6H14O  | 000994-05-8 | 78   |
| 2    |    | 2,2,4-Trimethyl-3-pentanol     | 130 | C8H18O  | 005162-48-1 | 39   |
| 3    |    | Silane, ethyltrimethyl-        | 102 | C5H14Si | 003439-38-1 | 28   |
| 4    |    | 2-Hydroxy-2-methylbutyric acid | 118 | C5H10O3 | 003739-30-8 | 25   |
| 5    |    | N-Ethylformamide               | 73  | C3H7NO  | 000627-45-2 | 9    |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
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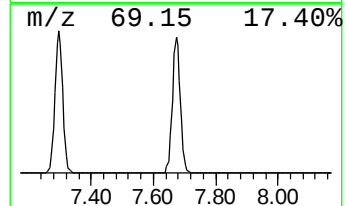
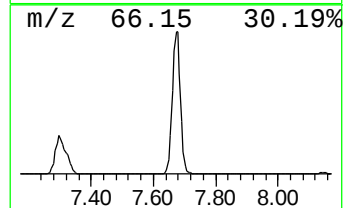
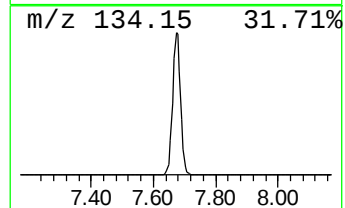
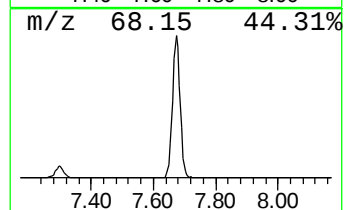
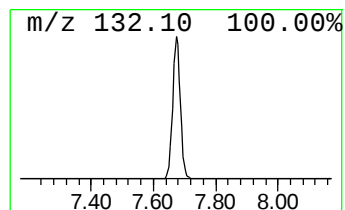
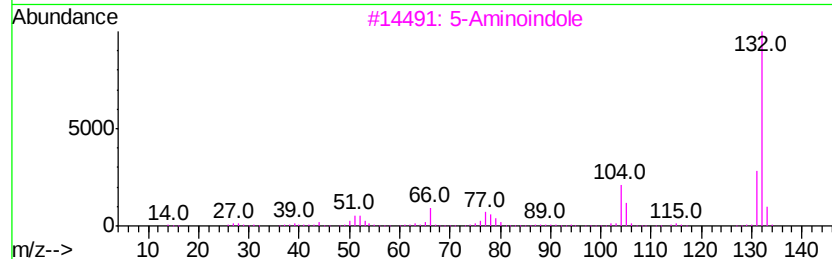
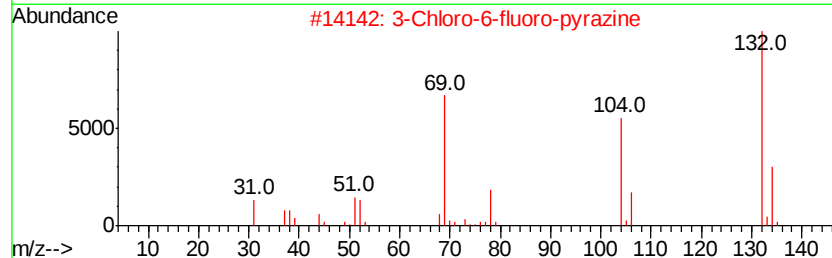
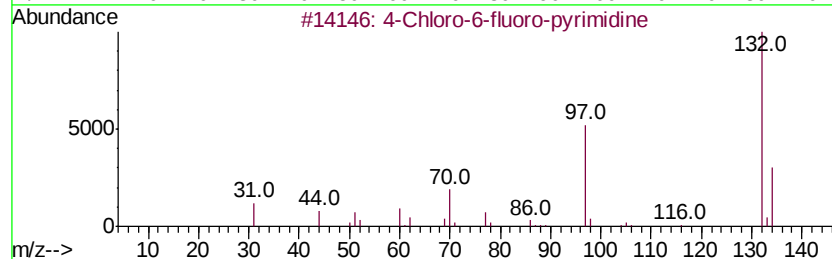
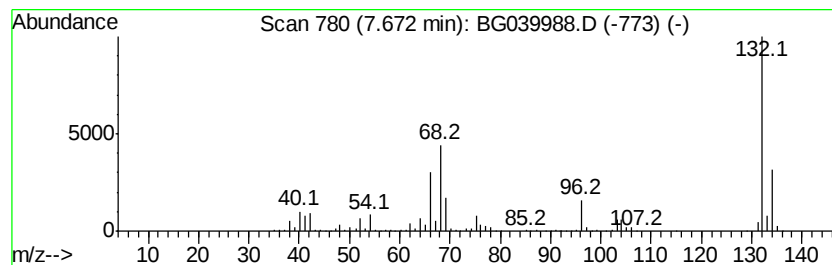
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown7.67 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.67 | 101.09 ng | 1302150 | 1,4-Dichlorobenzene-d4 | 8.15 |

| Hit# | of | Tentative ID                 | MW  | MolForm   | CAS#         | Qual |
|------|----|------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 4-Chloro-6-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-01-6  | 27   |
| 2    |    | 3-Chloro-6-fluoro-pyrazine   | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 3    |    | 5-Aminoindole                | 132 | C8H8N2    | 005192-03-0  | 22   |
| 4    |    | 1H-Benzimidazole, 2-methyl-  | 132 | C8H8N2    | 000615-15-6  | 22   |
| 5    |    | 5-Fluoro-2-chloropyrimidine  | 132 | C4H2ClFN2 | 062802-42-0  | 16   |



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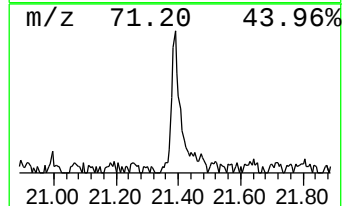
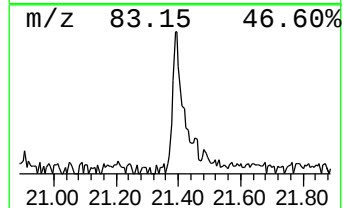
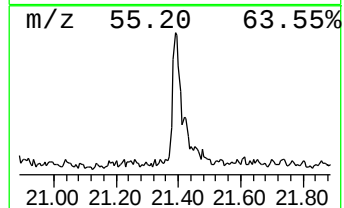
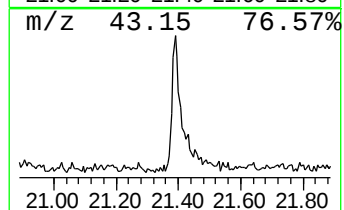
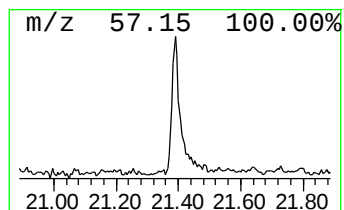
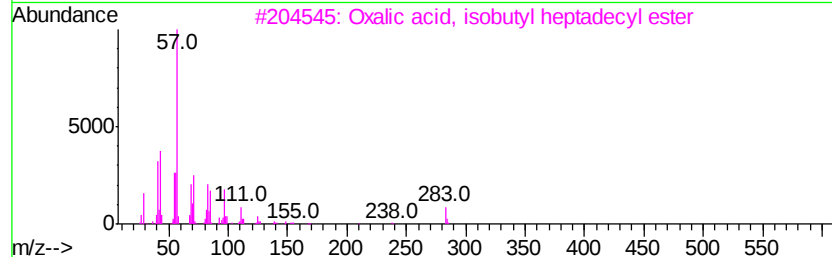
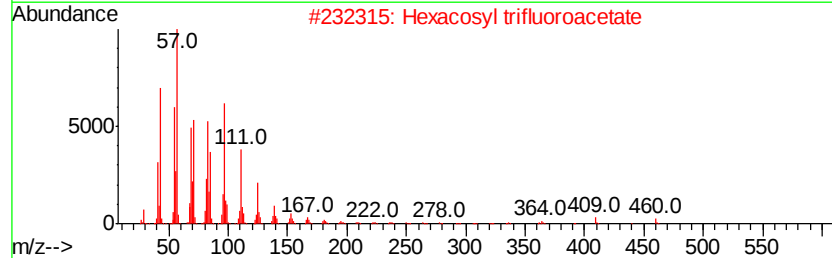
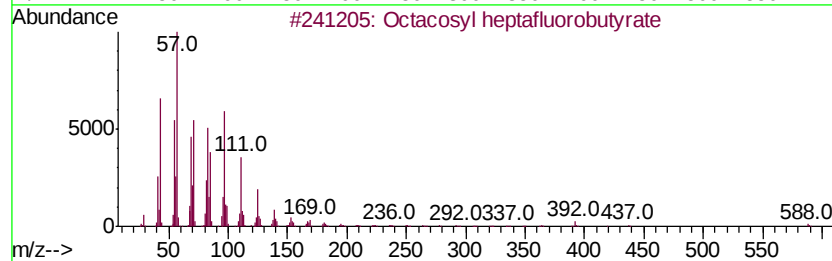
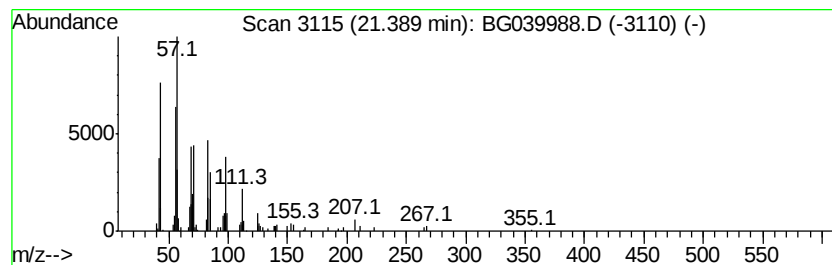
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octacosyl heptafluorobutyrate Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 21.39 | 3.14 ng | 128548 | Chrysene-d12     | 21.80 |

| Hit# of 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|-----------|-------------------------------------|-----|------------|--------------|------|
| 1         | Octacosyl heptafluorobutvrate       | 606 | C32H57F7O2 | 1000351-83-6 | 91   |
| 2         | Hexacosyl trifluoroacetate          | 478 | C28H53F3O2 | 1000351-75-0 | 91   |
| 3         | Oxalic acid, isobutyl heptadecyl... | 384 | C23H44O4   | 1000309-38-2 | 91   |
| 4         | Tetracosyl heptafluorobutvrate      | 550 | C28H49F7O2 | 1000351-83-7 | 91   |
| 5         | Heptacosyl pentafluoropropionate    | 542 | C30H55F5O2 | 1000351-81-6 | 91   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG030419.M  
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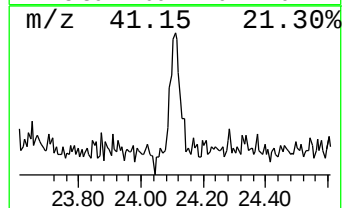
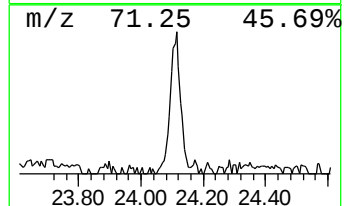
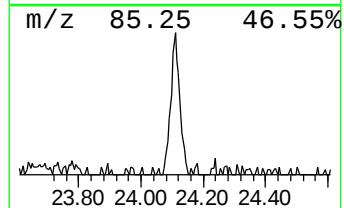
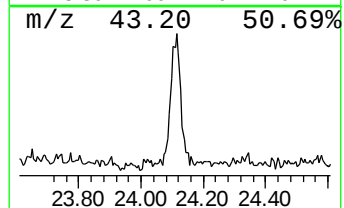
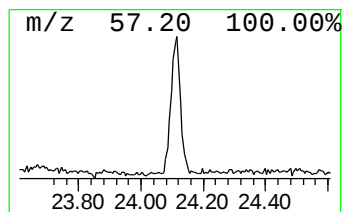
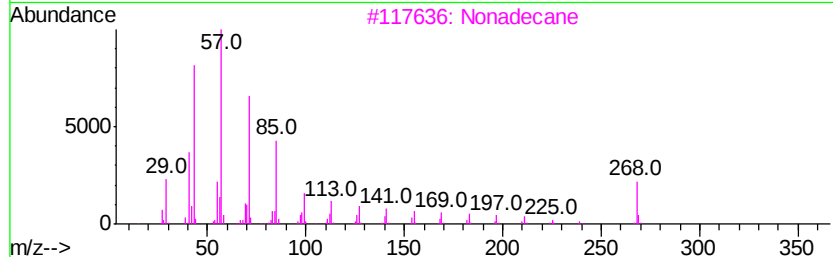
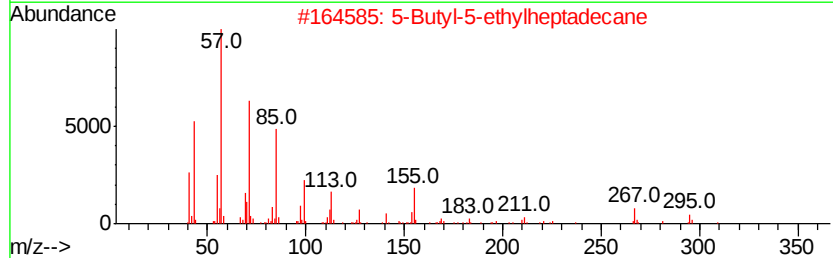
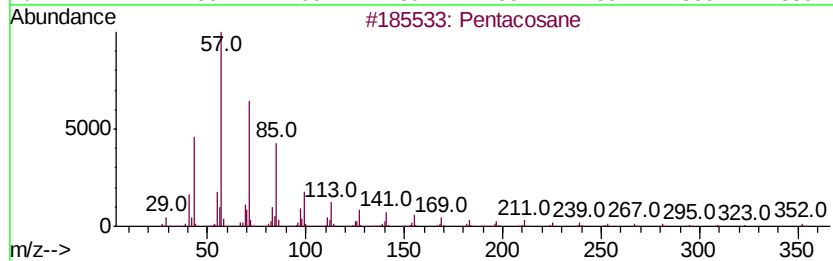
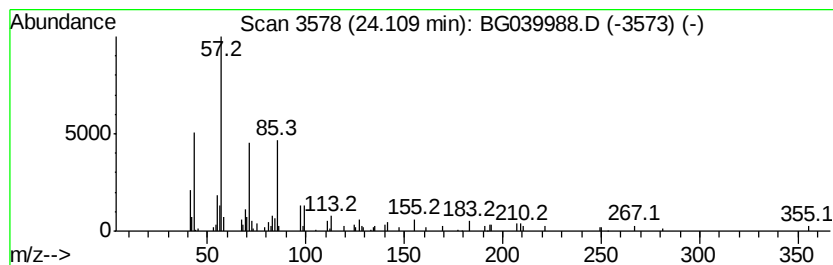
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Pentacosane Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 24.11 | 2.23 ng | 85524 | Perylene-d12     | 25.16 |

| Hit# of | 5                          | Tentative ID | MW  | MolForm | CAS#         | Qual |
|---------|----------------------------|--------------|-----|---------|--------------|------|
| 1       | Pentacosane                |              | 352 | C25H52  | 000629-99-2  | 87   |
| 2       | 5-Butyl-5-ethylheptadecane |              | 324 | C23H48  | 1000360-43-0 | 80   |
| 3       | Nonadecane                 |              | 268 | C19H40  | 000629-92-5  | 74   |
| 4       | Tetracosane                |              | 338 | C24H50  | 000646-31-1  | 72   |
| 5       | Pentadecane, 8-heptyl-     |              | 310 | C22H46  | 071005-15-7  | 72   |



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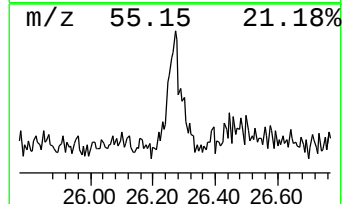
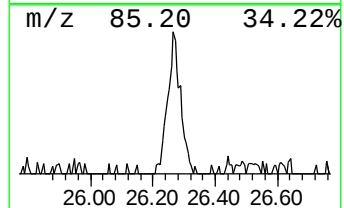
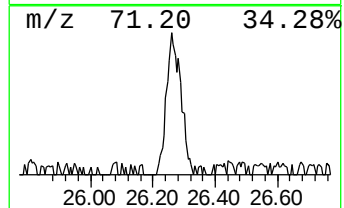
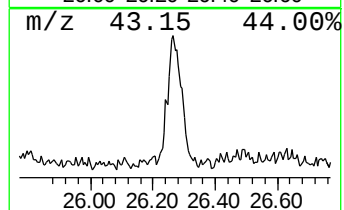
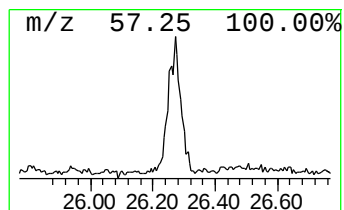
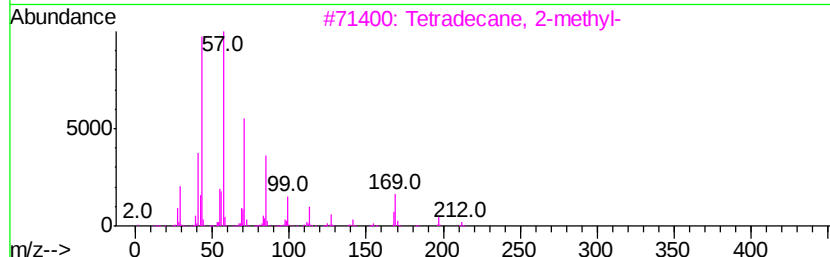
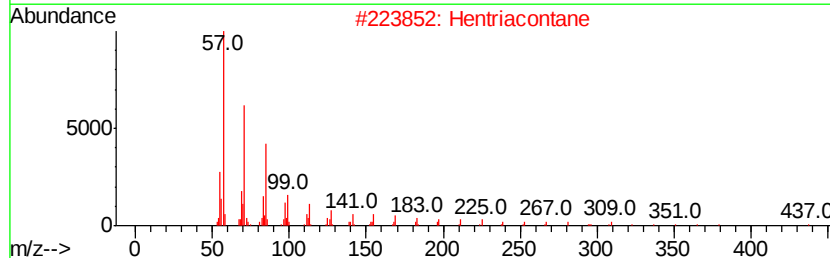
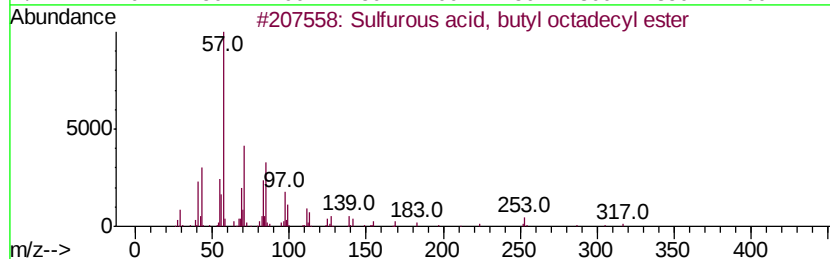
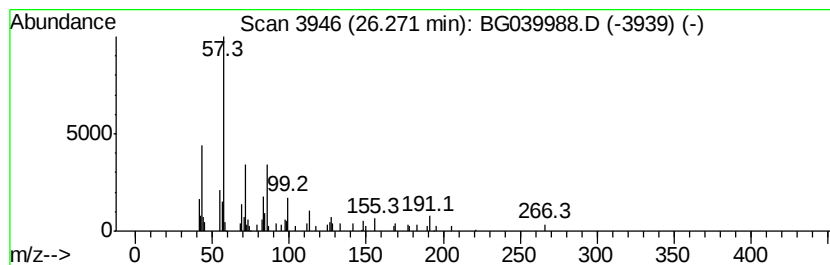
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Sulfurous acid, butyl octadecyl... Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 26.27 | 2.18 ng | 83615 | Perylene-d12     | 25.16 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Sulfurous acid, butyl octadecyl ... | 390 | C22H46O3S | 1000309-18-5 | 72   |
| 2    |    |   | Hentriacontane                      | 437 | C31H64    | 000630-04-6  | 53   |
| 3    |    |   | Tetradecane, 2-methyl-              | 212 | C15H32    | 001560-95-8  | 53   |
| 4    |    |   | Hexacosane                          | 366 | C26H54    | 000630-01-3  | 53   |
| 5    |    |   | Tetradecane, 2,6,10-trimethyl-      | 240 | C17H36    | 014905-56-7  | 53   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_G\DATA\BG031819\  
Data File : BG039988.D  
Acq On : 19 Mar 2019 3:09  
Operator : JU/SJ  
Sample : K1930-01  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_G  
ClientSampleId :  
TP-3

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_G\METHODS\8270-BG030419.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| Butane, 2-methoxy... | 3.27  | 15.2    | ng    | 195259   | 1                     | 8.15  | 257616 | 20.0 |
| unknown7.67          | 7.67  | 101.1   | ng    | 1302150  | 1                     | 8.15  | 257616 | 20.0 |
| Octacosyl heptafl... | 21.39 | 3.1     | ng    | 128548   | 5                     | 21.80 | 819123 | 20.0 |
| Pentacosane          | 24.11 | 2.2     | ng    | 85524    | 6                     | 25.16 | 766644 | 20.0 |
| Sulfurous acid, b... | 26.27 | 2.2     | ng    | 83615    | 6                     | 25.16 | 766644 | 20.0 |