

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022823\  
 Data File : BF132580.D  
 Acq On : 28 Feb 2023 19:29  
 Operator : CG\JU  
 Sample : 01701-05  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 EB-2023-2-24

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132580.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         | 4.640       | 345           | 349         | 355          | rBV      | 89055          | 95214         | 1.44%           | 0.248%        |
| 2         | 5.234       | 446           | 450         | 461          | rVB      | 1176870        | 1212524       | 18.35%          | 3.157%        |
| 3         | 5.622       | 512           | 516         | 527          | rBV      | 2429718        | 2398049       | 36.28%          | 6.244%        |
| 4         | 6.016       | 580           | 583         | 590          | rVB      | 143029         | 121800        | 1.84%           | 0.317%        |
| 5         | 6.622       | 682           | 686         | 691          | rBV      | 1488017        | 1393158       | 21.08%          | 3.628%        |
| 6         | 6.998       | 747           | 750         | 754          | rBV      | 1642102        | 1430143       | 21.64%          | 3.724%        |
| 7         | 7.569       | 841           | 847         | 850          | rBV      | 3812437        | 3757411       | 56.85%          | 9.784%        |
| 8         | 8.286       | 965           | 969         | 972          | rBV      | 2338833        | 1885223       | 28.52%          | 4.909%        |
| 9         | 8.492       | 1000          | 1004        | 1006         | rBV      | 88185          | 71849         | 1.09%           | 0.187%        |
| 10        | 8.516       | 1006          | 1008        | 1016         | rVB      | 114337         | 101154        | 1.53%           | 0.263%        |
| 11        | 9.363       | 1146          | 1152        | 1155         | rBV      | 6871833        | 6609192       | 100.00%         | 17.209%       |
| 12        | 9.469       | 1166          | 1170        | 1173         | rBV      | 517957         | 425096        | 6.43%           | 1.107%        |
| 13        | 10.051      | 1265          | 1269        | 1272         | rBV      | 2405335        | 2108992       | 31.91%          | 5.491%        |
| 14        | 10.286      | 1306          | 1309        | 1313         | rBV2     | 64595          | 73222         | 1.11%           | 0.191%        |
| 15        | 10.457      | 1333          | 1338        | 1342         | rBV5     | 126111         | 194987        | 2.95%           | 0.508%        |
| 16        | 10.592      | 1358          | 1361        | 1364         | rBV4     | 59167          | 73264         | 1.11%           | 0.191%        |
| 17        | 10.686      | 1373          | 1377        | 1379         | rBV      | 184752         | 224797        | 3.40%           | 0.585%        |
| 18        | 10.845      | 1399          | 1404        | 1407         | rBV      | 4618587        | 4333597       | 65.57%          | 11.284%       |
| 19        | 10.951      | 1418          | 1422        | 1425         | rBV      | 510324         | 549846        | 8.32%           | 1.432%        |
| 20        | 11.086      | 1443          | 1445        | 1448         | rBV3     | 97613          | 103343        | 1.56%           | 0.269%        |
| 21        | 11.422      | 1499          | 1502        | 1504         | rBV      | 290213         | 268006        | 4.06%           | 0.698%        |
| 22        | 11.545      | 1519          | 1523        | 1526         | rBV      | 2471250        | 2244135       | 33.95%          | 5.843%        |
| 23        | 13.139      | 1789          | 1794        | 1797         | rVB      | 6326469        | 6382834       | 96.58%          | 16.620%       |
| 24        | 14.204      | 1971          | 1975        | 1981         | rVB      | 1330118        | 1304335       | 19.74%          | 3.396%        |
| 25        | 15.751      | 2233          | 2238        | 2247         | rVB      | 717339         | 944044        | 14.28%          | 2.458%        |
| 26        | 16.509      | 2363          | 2367        | 2376         | rVB6     | 43816          | 99096         | 1.50%           | 0.258%        |

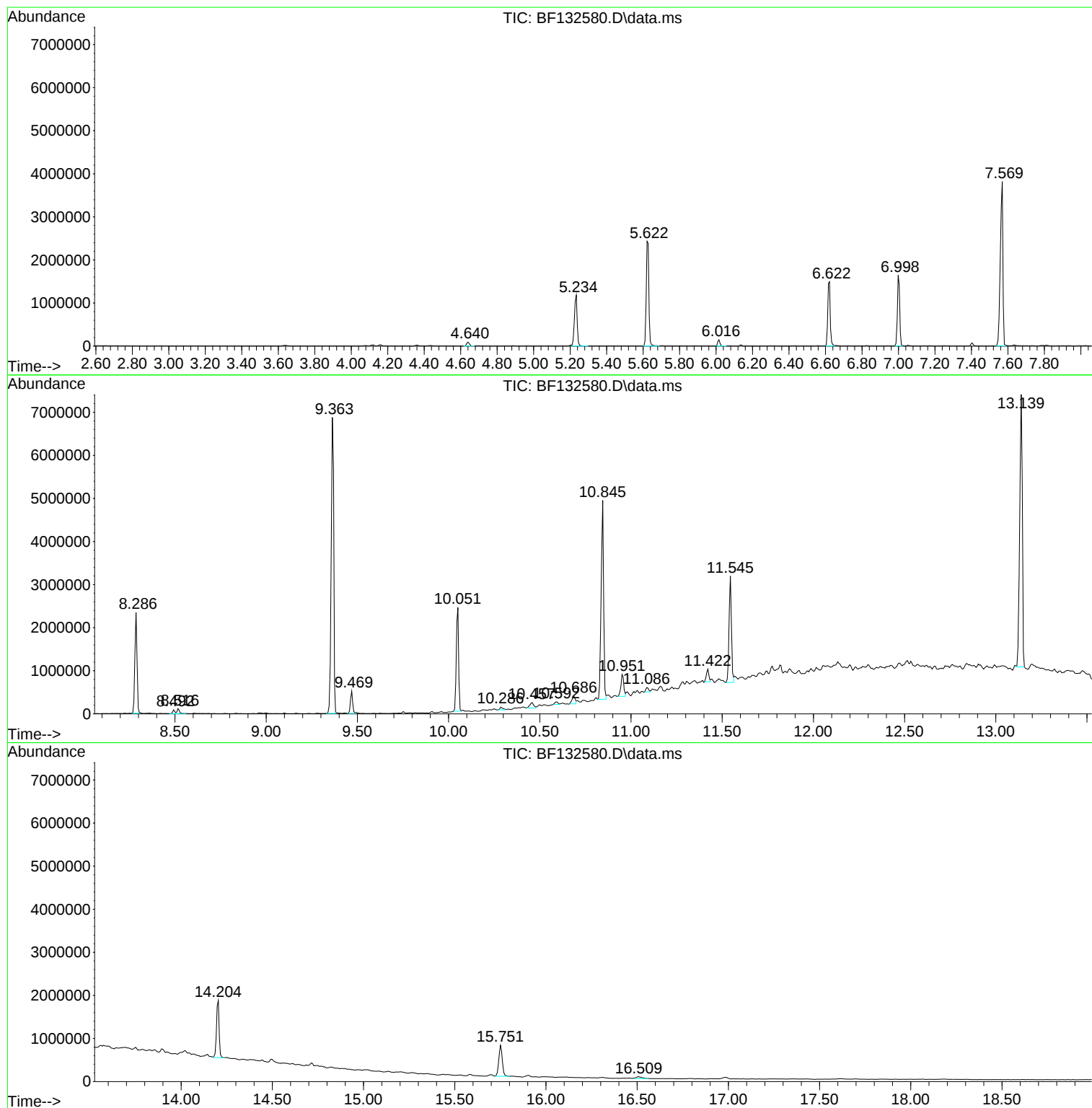
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ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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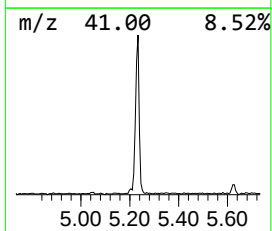
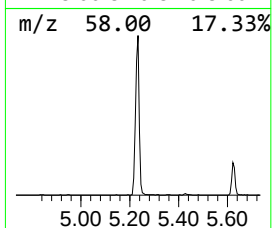
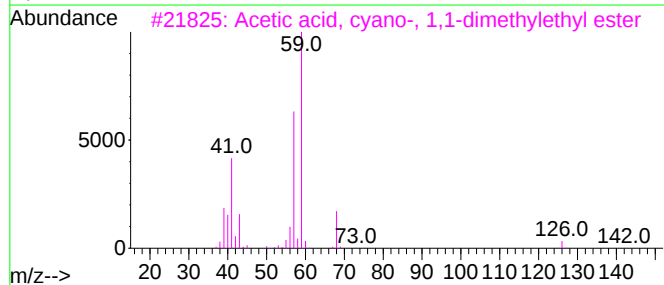
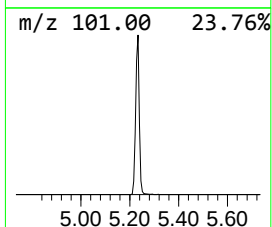
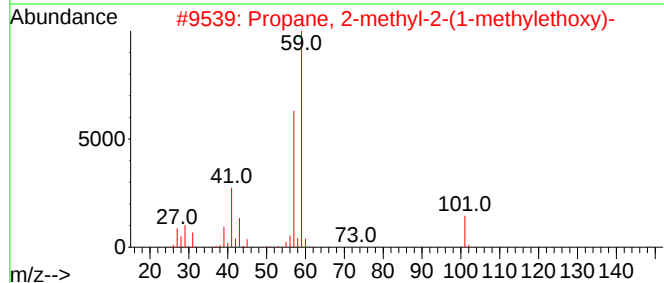
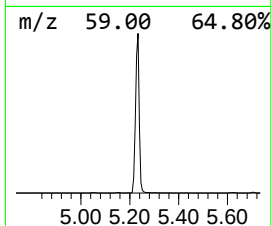
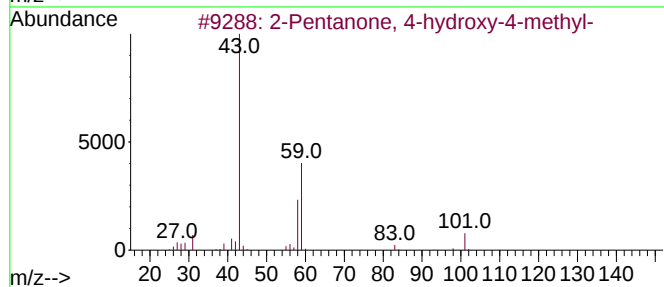
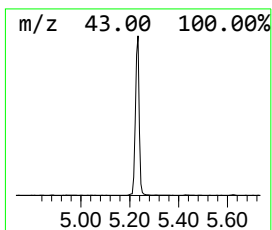
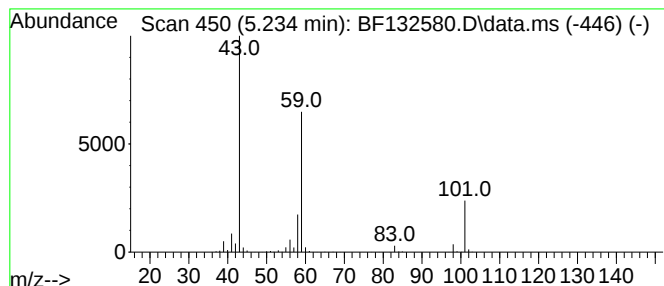
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

| R.T.  | EstConc  | Area    | Relative to ISTD       | R.T.  |
|-------|----------|---------|------------------------|-------|
| 5.234 | 16.96 ng | 1212520 | 1,4-Dichlorobenzene-d4 | 6.998 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 56      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 50      |      |      |
| 3    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2     | 001116-98-9 | 17      |      |      |
| 4    | 5-Hexen-2-one                       | 98  | C6H10O       | 000109-49-9 | 9       |      |      |
| 5    | Guanidine                           | 59  | CH5N3        | 000113-00-8 | 9       |      |      |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

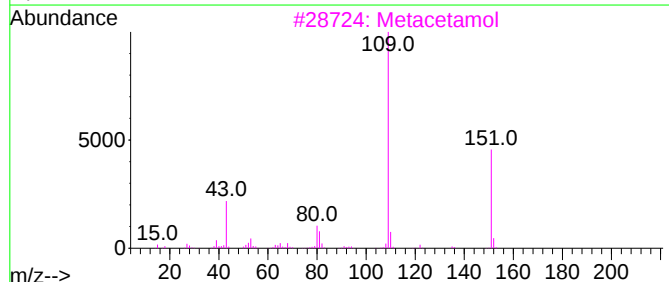
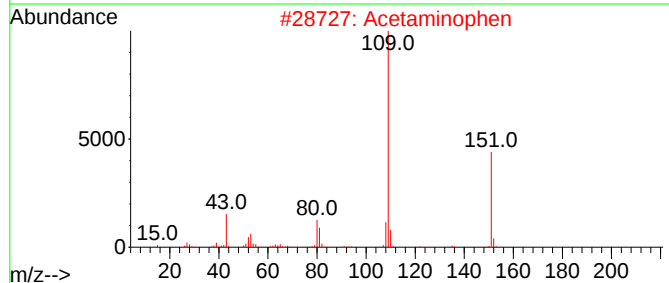
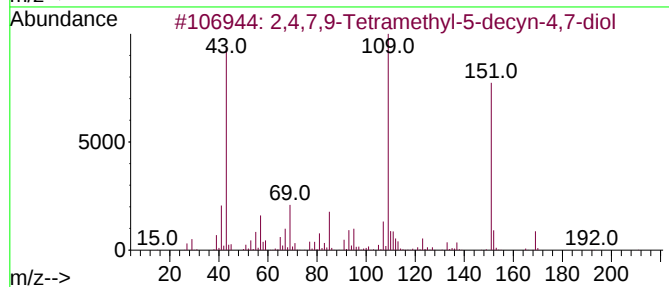
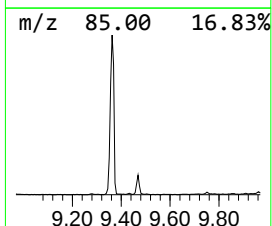
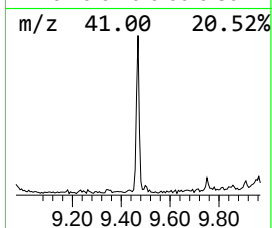
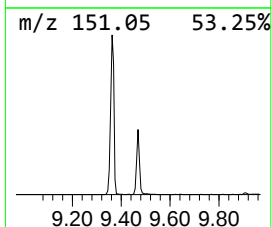
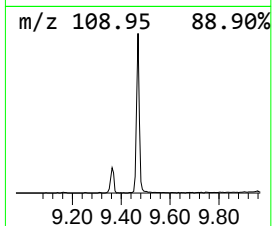
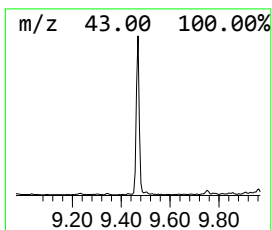
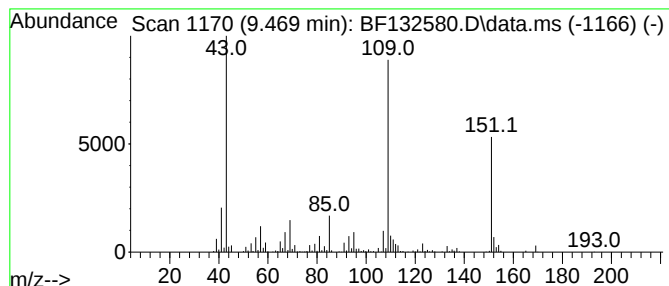
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.   |
|-------|---------|--------|------------------|--------|
| 9.469 | 4.03 ng | 425096 | Acenaphthene-d10 | 10.051 |

| Hit# | of 5                                | Tentative ID | MW       | MolForm | CAS#        | Qual |
|------|-------------------------------------|--------------|----------|---------|-------------|------|
| 1    | 2,4,7,9-Tetramethyl-5-decyn-4,7-... | 226          | C14H26O2 |         | 000126-86-3 | 68   |
| 2    | Acetaminophen                       | 151          | C8H9NO2  |         | 000103-90-2 | 59   |
| 3    | Metacetamol                         | 151          | C8H9NO2  |         | 000621-42-1 | 59   |
| 4    | Pyridine, 2-butyl-, 1-oxide         | 151          | C9H13NO  |         | 031396-32-4 | 45   |
| 5    | Ethanone, 1-(1,3-dimethyl-3-cycl... | 152          | C10H16O  |         | 051733-68-7 | 38   |



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Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
EB-2023-2-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

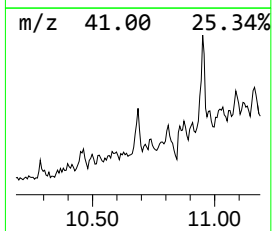
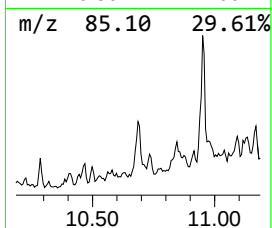
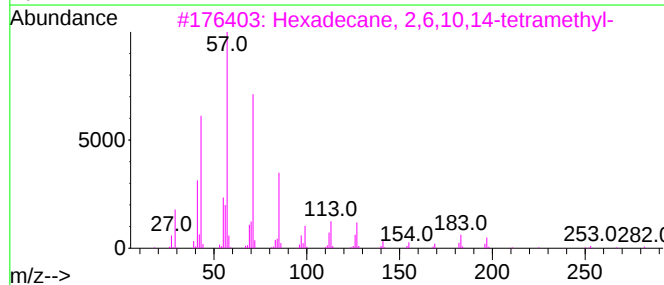
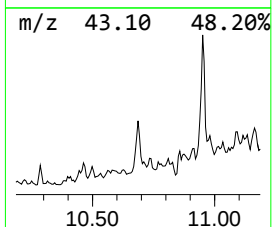
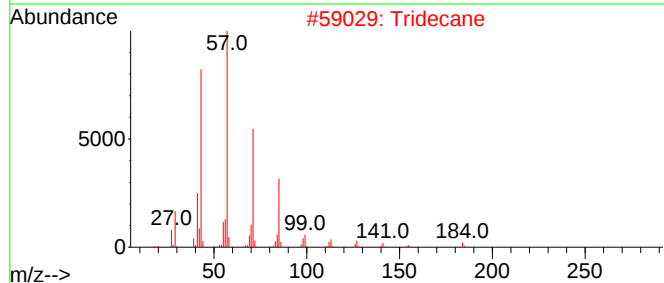
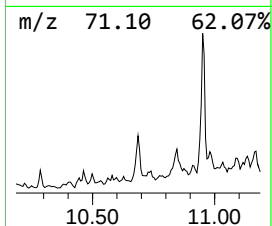
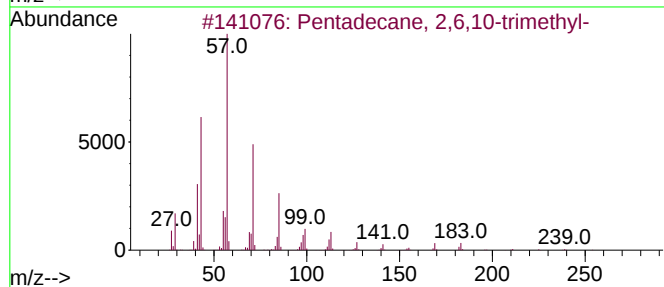
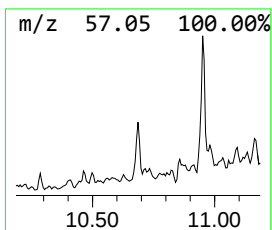
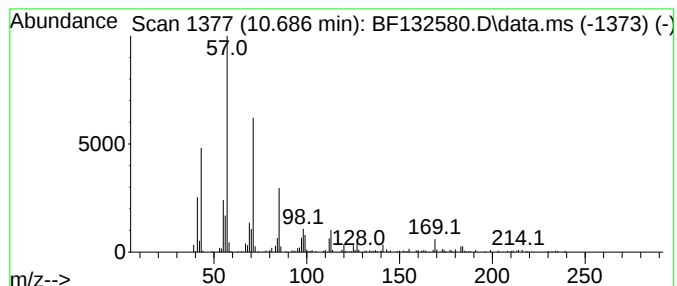
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Pentadecane, 2,6,10-trimethyl- Concentration Rank 5

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 10.686 | 2.13 ng | 224797 | Acenaphthene-d10 | 10.051 |

| Hit# | of | 5 | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|---|------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Pentadecane, 2,6,10-trimethyl-     | 254 | C18H38  | 003892-00-0 | 86   |
| 2    |    |   | Tridecane                          | 184 | C13H28  | 000629-50-5 | 81   |
| 3    |    |   | Hexadecane, 2,6,10,14-tetramethyl- | 282 | C20H42  | 000638-36-8 | 64   |
| 4    |    |   | Heptacosane                        | 380 | C27H56  | 000593-49-7 | 64   |
| 5    |    |   | Dodecane, 2-methyl-8-propyl-       | 226 | C16H34  | 055045-07-3 | 64   |



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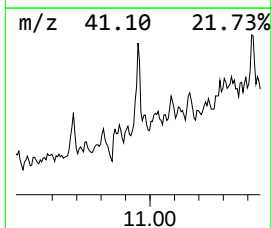
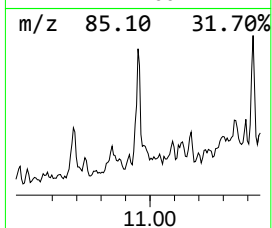
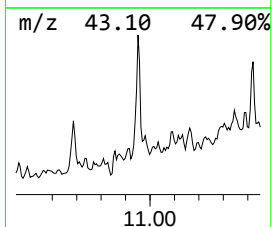
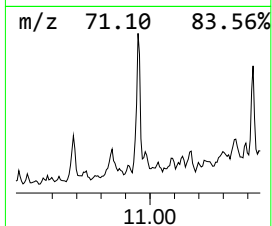
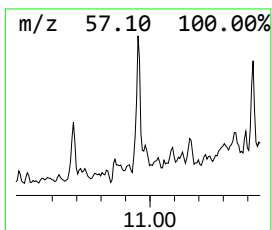
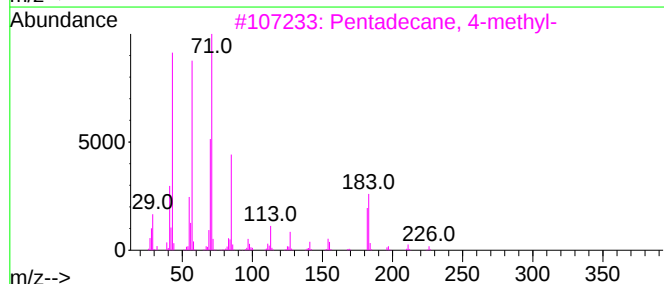
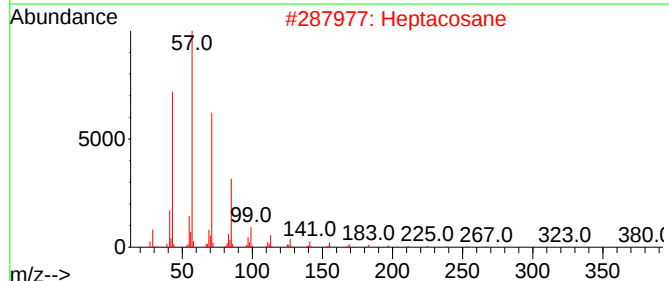
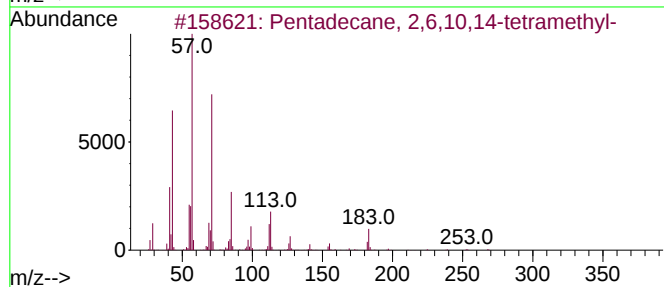
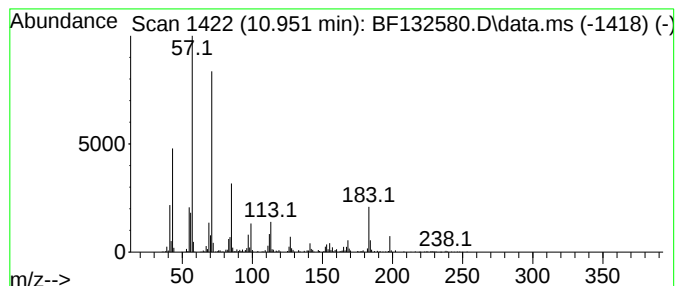
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Peak Number 4 Pentadecane, 2,6,10,14-tetr... Concentration Rank 2

| R.T.      | EstConc                             | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------------------------|--------|------------------|-------------|------|
| 10.951    | 4.90 ng                             | 549846 | Phenanthrene-d10 | 11.545      |      |
| Hit# of 5 | Tentative ID                        | MW     | MolForm          | CAS#        | Qual |
| 1         | Pentadecane, 2,6,10,14-tetramethyl- | 268    | C19H40           | 001921-70-6 | 72   |
| 2         | Heptacosane                         | 380    | C27H56           | 000593-49-7 | 72   |
| 3         | Pentadecane, 4-methyl-              | 226    | C16H34           | 002801-87-8 | 72   |
| 4         | Decane, 2-methyl-                   | 156    | C11H24           | 006975-98-0 | 68   |
| 5         | Tridecane                           | 184    | C13H28           | 000629-50-5 | 68   |



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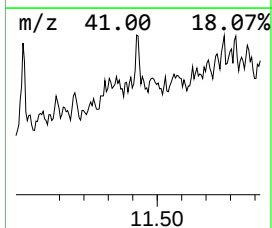
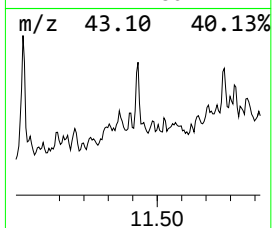
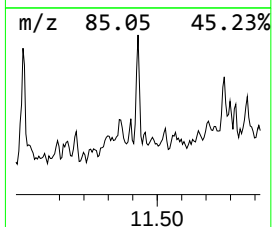
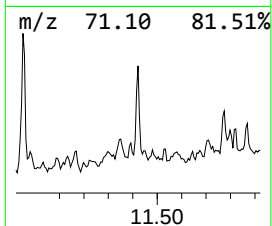
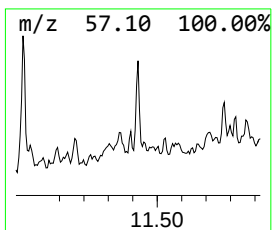
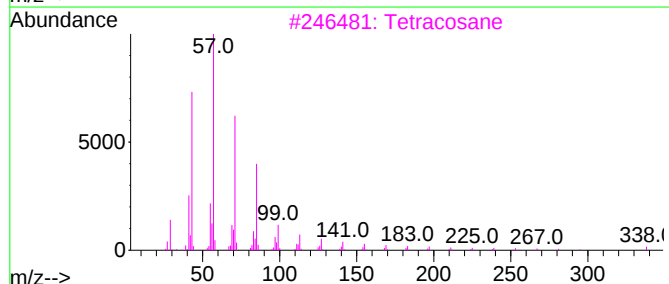
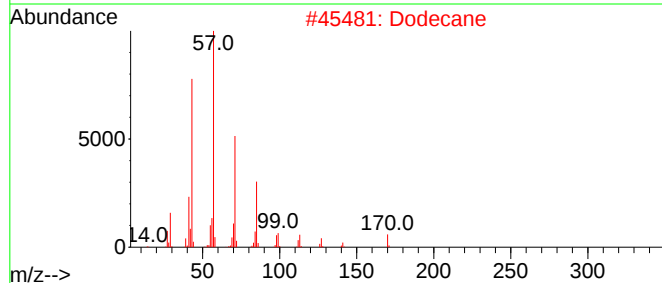
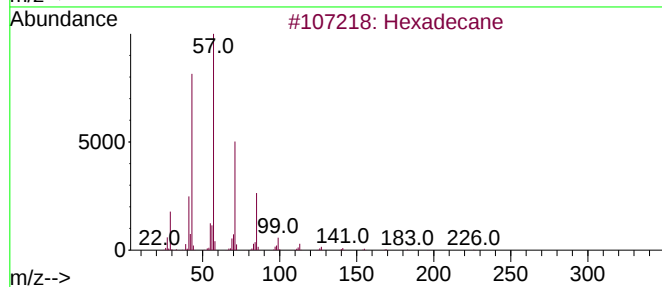
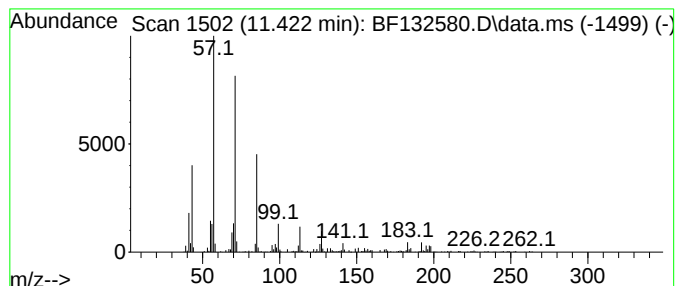
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexadecane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.422 | 2.39 ng | 268006 | Phenanthrene-d10 | 11.545 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Hexadecane           | 226 | C16H34  | 000544-76-3 | 93   |
| 2    |    |   | Dodecane             | 170 | C12H26  | 000112-40-3 | 90   |
| 3    |    |   | Tetracosane          | 338 | C24H50  | 000646-31-1 | 78   |
| 4    |    |   | Tridecane, 1-iodo-   | 310 | C13H27I | 035599-77-0 | 78   |
| 5    |    |   | Tetradecane, 1-iodo- | 324 | C14H29I | 019218-94-1 | 78   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022823\  
Data File : BF132580.D  
Acq On : 28 Feb 2023 19:29  
Operator : CG\JU  
Sample : 01701-05  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
EB-2023-2-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

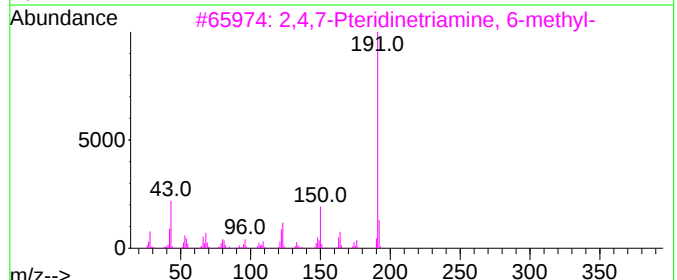
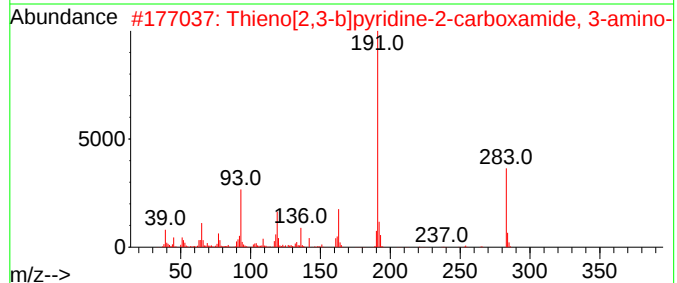
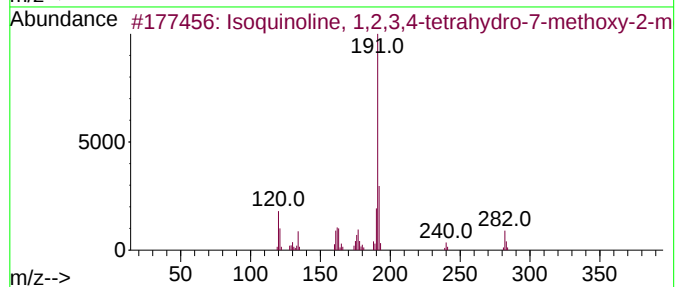
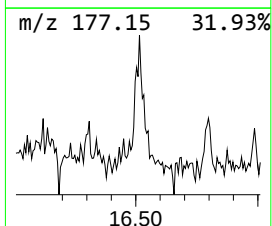
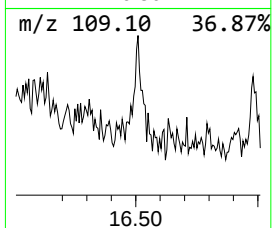
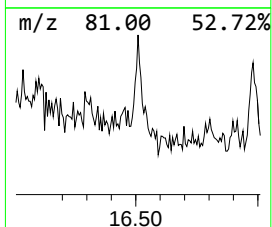
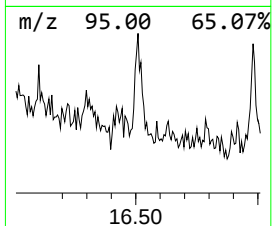
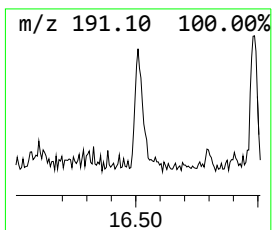
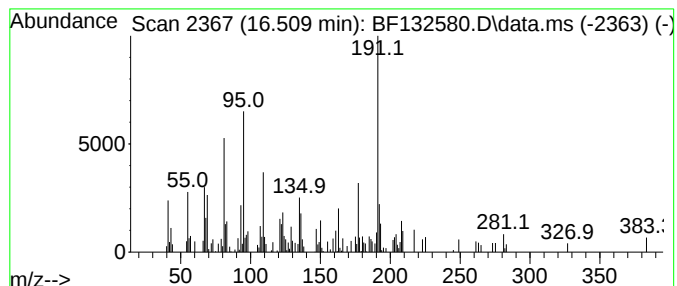
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 unknown16.509 Concentration Rank 6

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 16.509 | 2.10 ng | 99096 | Perylene-d12     | 15.751 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|------------|--------------|------|
| 1    |    |   | Isoquinoline, 1,2,3,4-tetrahydro... | 283 | C18H21NO2  | 036646-87-4  | 47   |
| 2    |    |   | Thieno[2,3-b]pyridine-2-carboxam... | 283 | C15H13N3OS | 1000350-91-6 | 38   |
| 3    |    |   | 2,4,7-Pteridinetriamine, 6-methyl-  | 191 | C7H9N7     | 017539-50-3  | 38   |
| 4    |    |   | 2-Aminoxymethylphenanthrene         | 223 | C15H13NO   | 1010426-07-2 | 38   |
| 5    |    |   | Anthracene, 9-dodecyltetradecahy... | 360 | C26H48     | 055401-75-7  | 38   |



Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF022823\  
Data File : BF132580.D  
Acq On : 28 Feb 2023 19:29  
Operator : CG\JU  
Sample : 01701-05  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
EB-2023-2-24

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF022223.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 |
| 2-Pentanone, 4-... | 5.234  | 17.0    | ng    | 1212520  | 1                     | 6.998  | 1430140 | 20.0 |
| 2,4,7,9-Tetrame... | 9.469  | 4.0     | ng    | 425096   | 3                     | 10.051 | 2108990 | 20.0 |
| Pentadecane, 2,... | 10.686 | 2.1     | ng    | 224797   | 3                     | 10.051 | 2108990 | 20.0 |
| Pentadecane, 2,... | 10.951 | 4.9     | ng    | 549846   | 4                     | 11.545 | 2244140 | 20.0 |
| Hexadecane         | 11.422 | 2.4     | ng    | 268006   | 4                     | 11.545 | 2244140 | 20.0 |
| unknown16.509      | 16.509 | 2.1     | ng    | 99096    | 6                     | 15.751 | 944044  | 20.0 |