

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF072423\  
 Data File : BF134442.D  
 Acq On : 24 Jul 2023 22:17  
 Operator : CG\JU  
 Sample : 03670-01  
 Misc :  
 ALS Vial : 6 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 N48909

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-BF072423.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134442.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         | 5.463       | 571           | 574         | 582          | rBV      | 488187         | 483515        | 16.61%          | 6.315%        |
| 2         | 6.469       | 742           | 745         | 755          | rBV      | 281865         | 298245        | 10.25%          | 3.895%        |
| 3         | 6.834       | 804           | 807         | 812          | rBV      | 350871         | 291012        | 10.00%          | 3.801%        |
| 4         | 7.398       | 899           | 903         | 906          | rBV      | 852037         | 693824        | 23.84%          | 9.061%        |
| 5         | 8.110       | 1022          | 1024        | 1028         | rVB      | 440796         | 360616        | 12.39%          | 4.710%        |
| 6         | 8.569       | 1100          | 1102        | 1105         | rVB3     | 122915         | 110454        | 3.80%           | 1.443%        |
| 7         | 8.651       | 1112          | 1116        | 1118         | rBV3     | 68909          | 104215        | 3.58%           | 1.361%        |
| 8         | 8.733       | 1126          | 1130        | 1132         | rBV4     | 86223          | 148322        | 5.10%           | 1.937%        |
| 9         | 8.798       | 1138          | 1141        | 1148         | rVB7     | 94290          | 153342        | 5.27%           | 2.003%        |
| 10        | 8.851       | 1148          | 1150        | 1153         | rBV2     | 106143         | 119776        | 4.12%           | 1.564%        |
| 11        | 9.198       | 1204          | 1209        | 1216         | rBV      | 780174         | 1555415       | 53.45%          | 20.313%       |
| 12        | 14.680      | 2138          | 2141        | 2161         | rVB      | 2015319        | 2910204       | 100.00%         | 38.007%       |
| 13        | 15.568      | 2288          | 2292        | 2298         | rVB      | 298861         | 428113        | 14.71%          | 5.591%        |

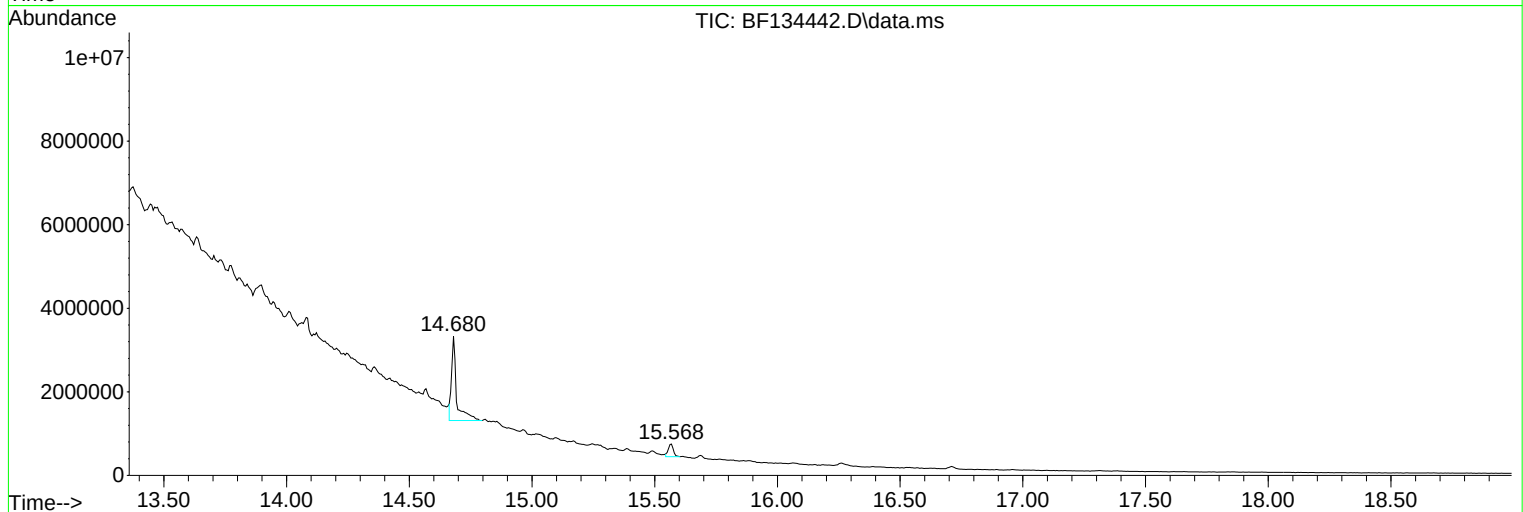
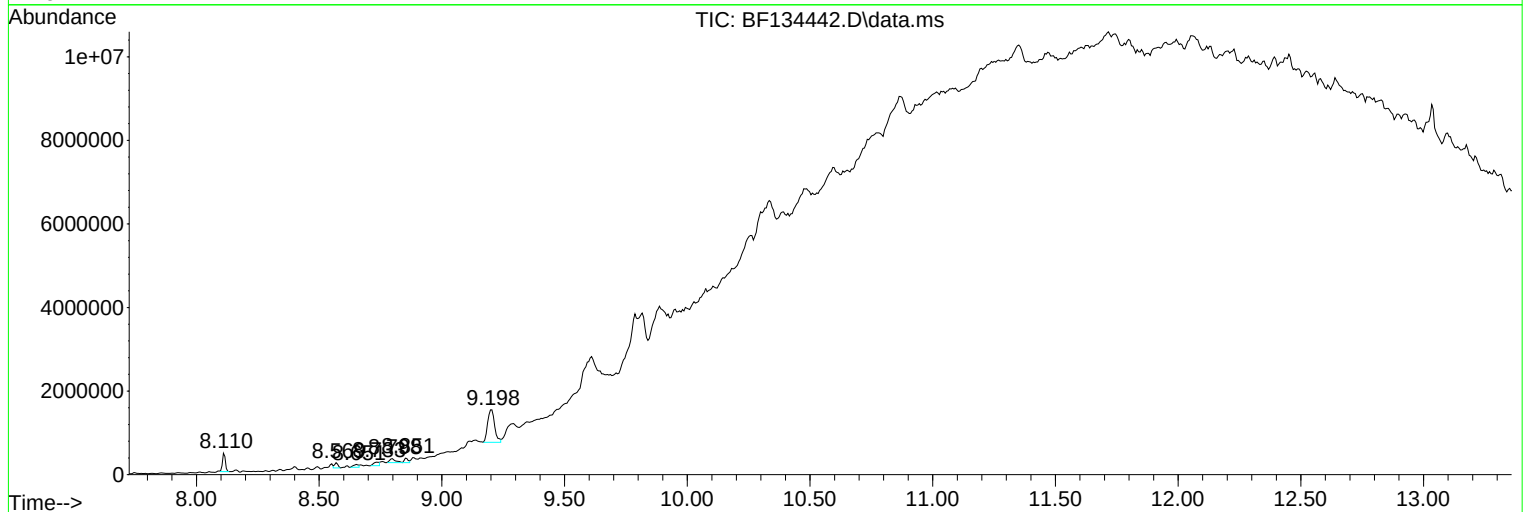
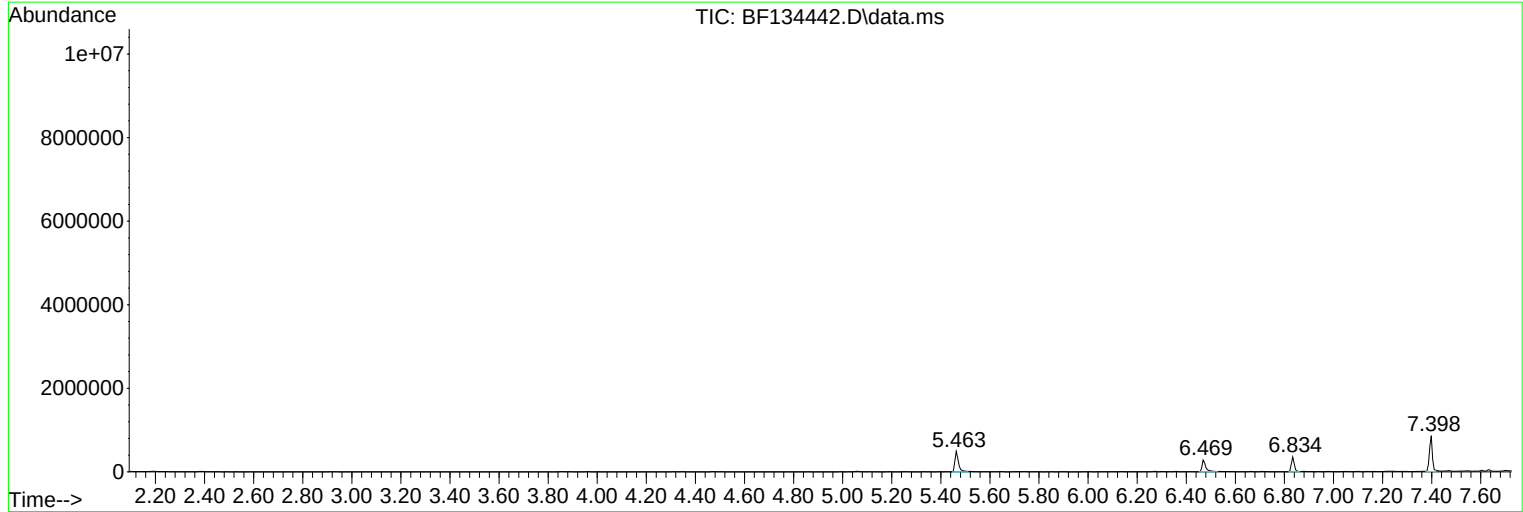
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ALS Vial : 6 Sample Multiplier: 1

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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072423.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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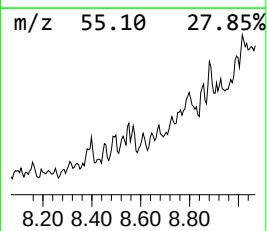
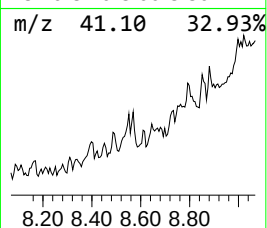
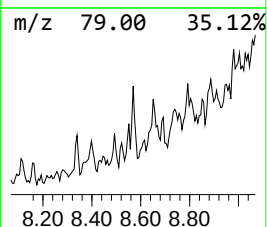
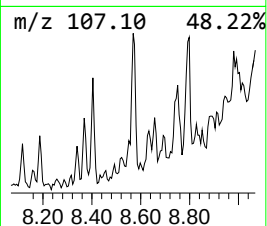
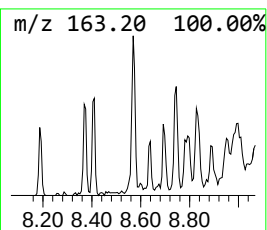
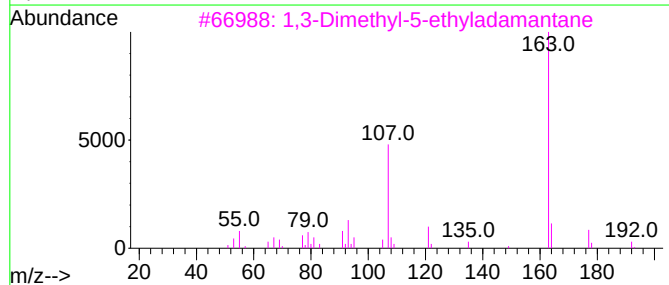
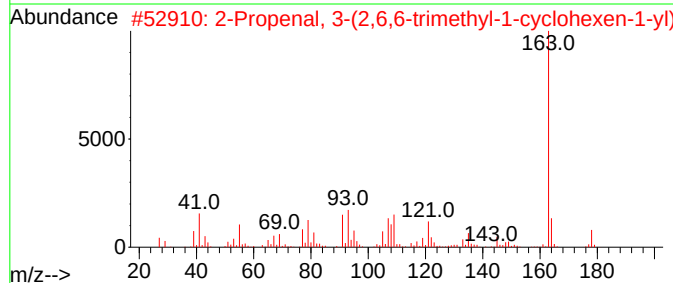
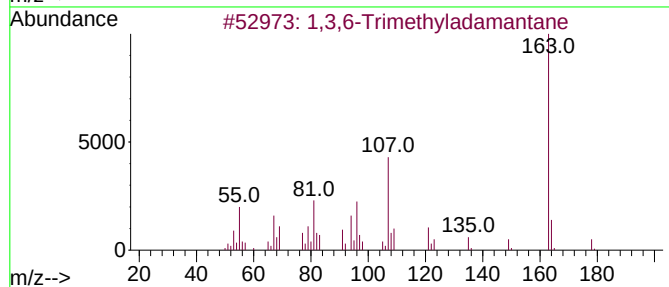
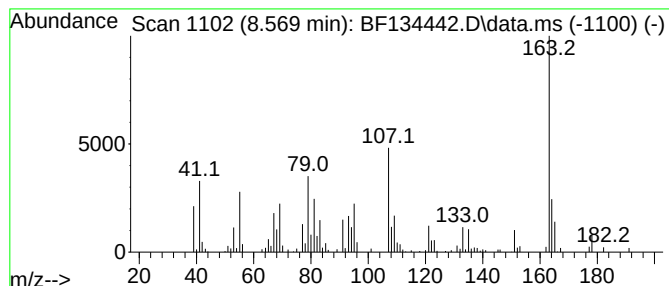
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072423.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 1,3,6-Trimethyladamantane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.569 | 6.13 ng | 110454 | Naphthalene-d8   | 8.110 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 1,3,6-Trimethyladamantane           | 178 | C13H22   | 024139-37-5 | 64   |
| 2    |    |   | 2-Propenal, 3-(2,6,6-trimethyl-1... | 178 | C12H18O  | 004951-40-0 | 60   |
| 3    |    |   | 1,3-Dimethyl-5-ethyladamantane      | 192 | C14H24   | 001687-35-0 | 50   |
| 4    |    |   | 1,3,5-Trimethyladamantane           | 178 | C13H22   | 000707-35-7 | 50   |
| 5    |    |   | Tricyclo[3.3.1.1(3,7)-]decane, 1... | 242 | C12H19Br | 000941-37-7 | 50   |



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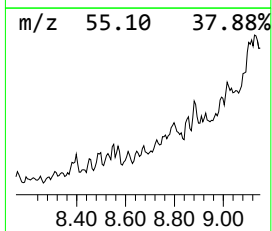
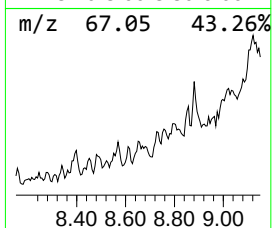
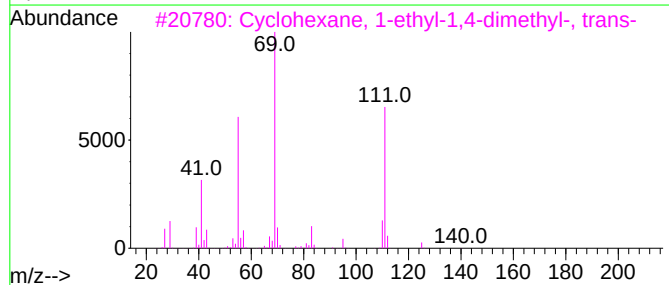
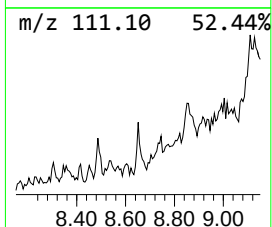
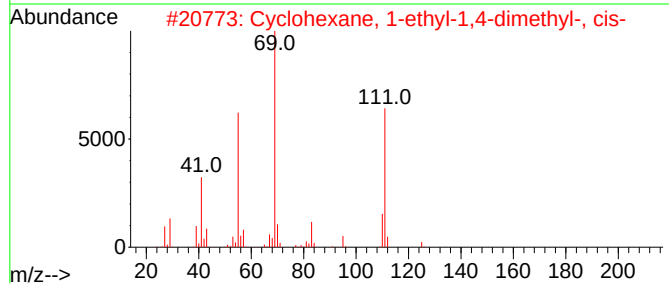
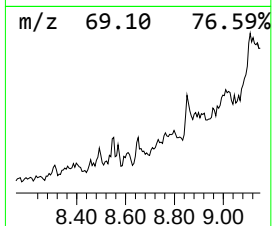
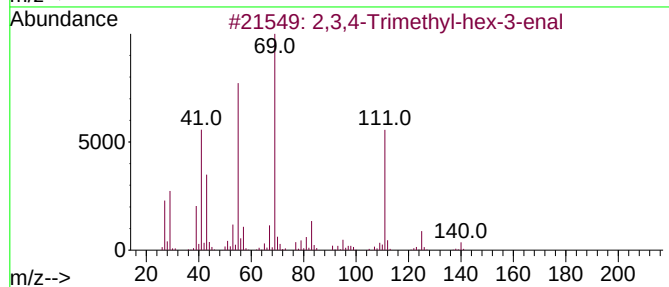
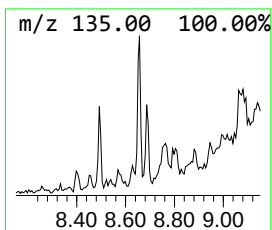
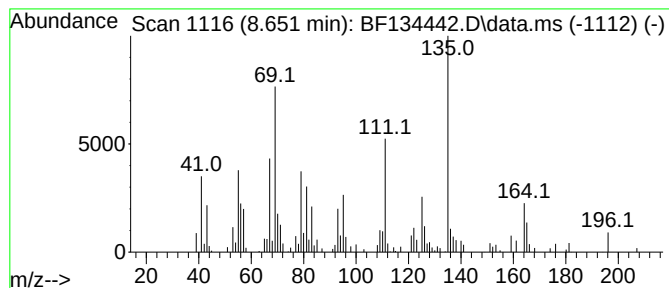
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072423.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 unknown8.651 Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.651 | 5.78 ng | 104215 | Naphthalene-d8   | 8.110 |

| Hit# | of 5 | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|------|-------------------------------------|-----|---------|--------------|------|
| 1    |      | 2,3,4-Trimethyl-hex-3-enal          | 140 | C9H16O  | 1000193-72-9 | 30   |
| 2    |      | Cyclohexane, 1-ethyl-1,4-dimethy... | 140 | C10H20  | 062238-30-6  | 27   |
| 3    |      | Cyclohexane, 1-ethyl-1,4-dimethy... | 140 | C10H20  | 062238-32-8  | 27   |
| 4    |      | Cyclopentane, 1,1,3-trimethyl-3-... | 166 | C12H22  | 074421-09-3  | 27   |
| 5    |      | Cyclooctane, ethyl-                 | 140 | C10H20  | 013152-02-8  | 25   |



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ALS Vial : 6 Sample Multiplier: 1

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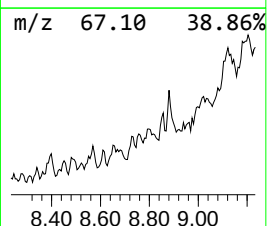
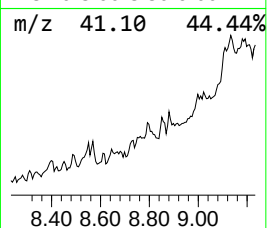
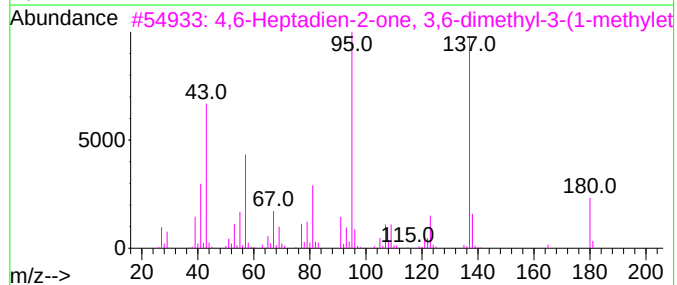
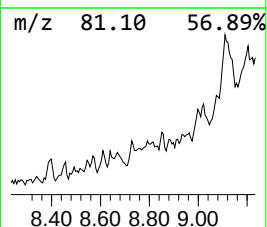
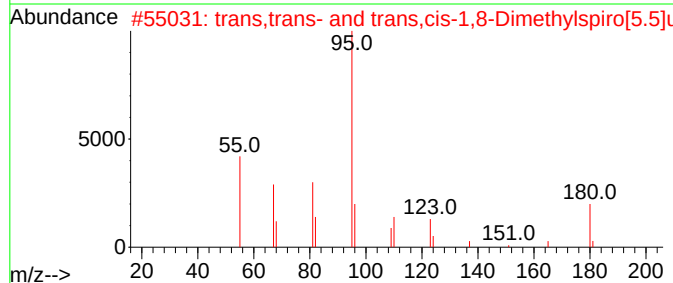
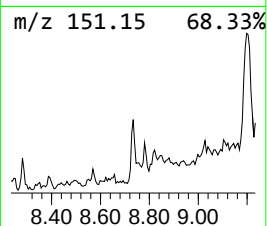
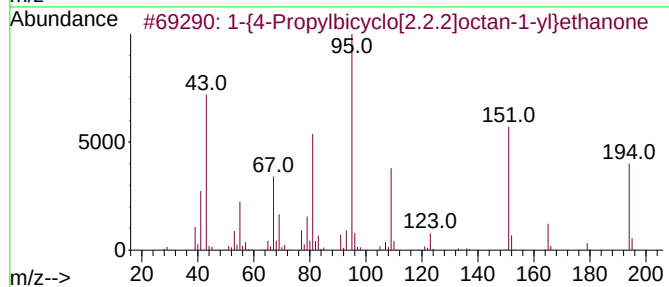
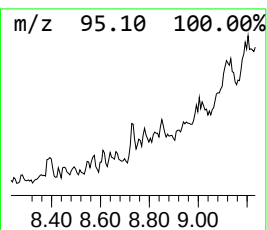
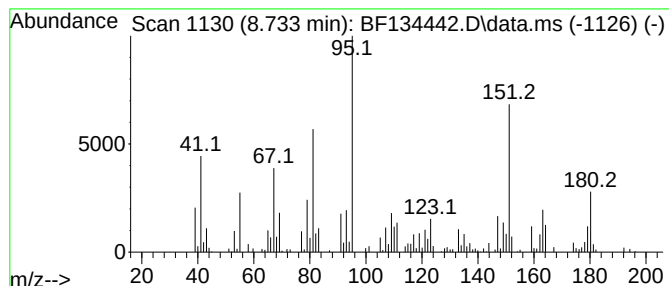
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072423.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown8.733 Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.733 | 8.23 ng | 148322 | Naphthalene-d8   | 8.110 |

| Hit# | of                   | 5 | Tentative ID                      | MW  | MolForm | CAS#         | Qual |
|------|----------------------|---|-----------------------------------|-----|---------|--------------|------|
| 1    | 1                    |   | {4-Propylbicyclo[2.2.2]octan-1... | 194 | C13H22O | 1000435-24-0 | 47   |
| 2    | trans,trans-         |   | and trans,cis-1,8-D...            | 180 | C13H24  | 1000111-73-2 | 46   |
| 3    | 4,6-Heptadien-2-one, |   | 3,6-dimethy...                    | 180 | C12H20O | 077822-50-5  | 42   |
| 4    | 5-Octen-2-yn-4-ol    |   |                                   | 124 | C8H12O  | 1010196-87-1 | 38   |
| 5    | Ketone,              |   | 1,5-dimethylbicyclo[2.1....       | 138 | C9H14O  | 024081-57-0  | 35   |



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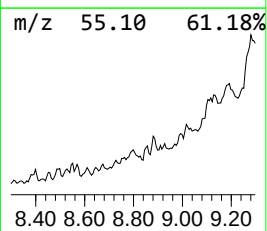
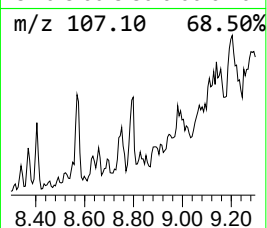
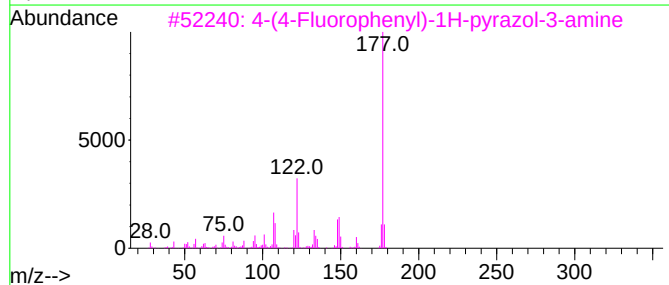
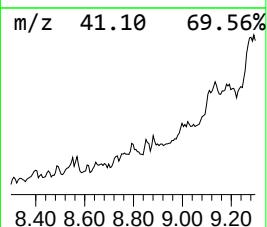
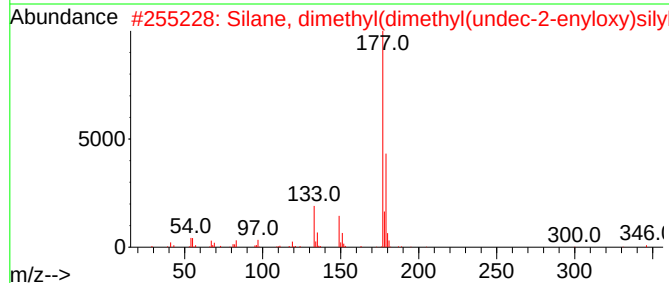
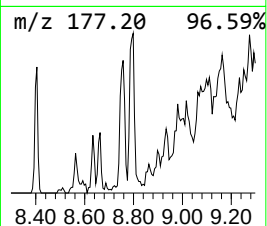
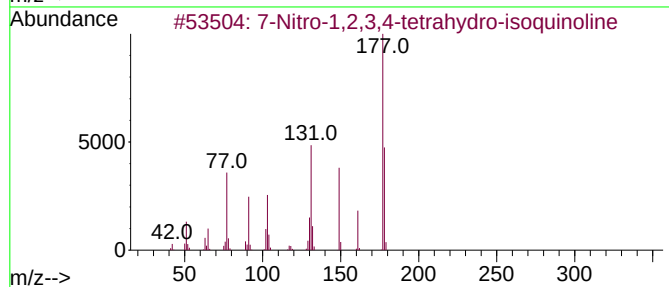
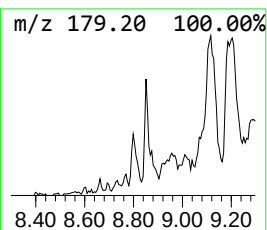
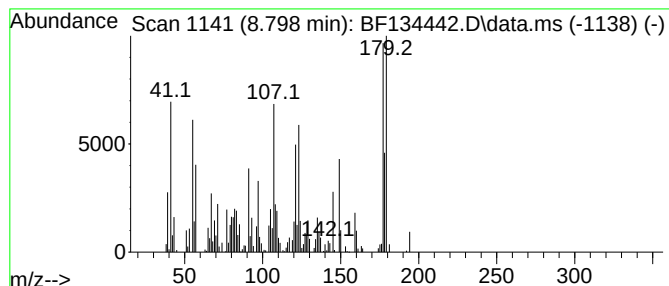
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown8.798 Concentration Rank 1

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.798 | 8.50 ng | 153342 | Naphthalene-d8   | 8.110 |

| Hit# | of 5                                | Tentative ID | MW          | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|-------------|--------------|------|------|
| 1    | 7-Nitro-1,2,3,4-tetrahydro-isoqu... | 178          | C9H10N2O2   | 1000318-52-7 | 27   |      |
| 2    | Silane, dimethyl(dimethyl(undec-... | 346          | C17H38O3Si2 | 1000347-94-8 | 27   |      |
| 3    | 4-(4-Fluorophenyl)-1H-pyrazol-3-... | 177          | C9H8FN3     | 005848-04-4  | 22   |      |
| 4    | 4-(2-Thienyl)-2-pyrimidinylamine    | 177          | C8H7N3S     | 154321-60-5  | 18   |      |
| 5    | Silane, tributylchloro-             | 234          | C12H27ClSi  | 000995-45-9  | 14   |      |



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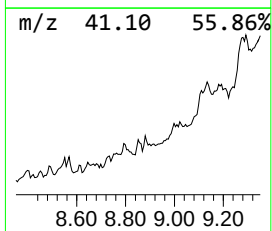
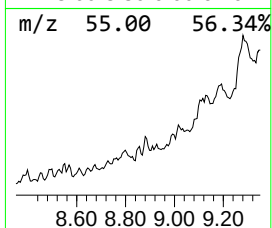
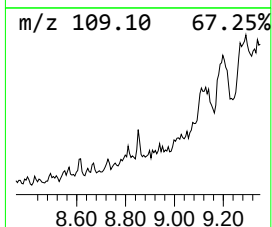
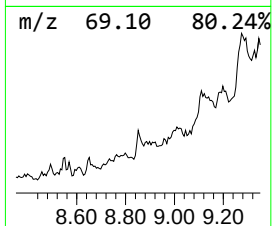
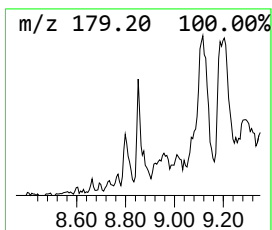
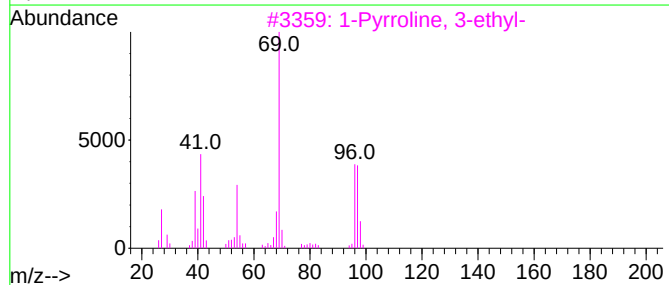
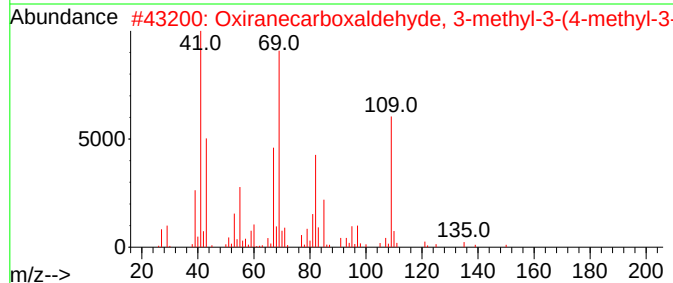
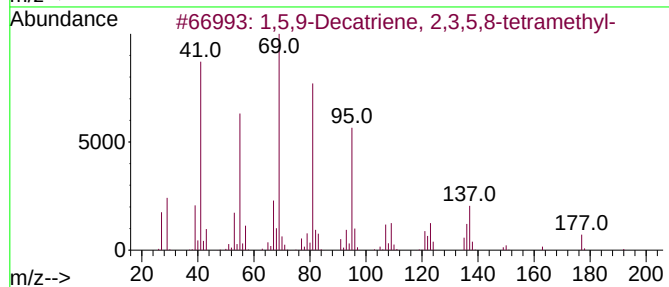
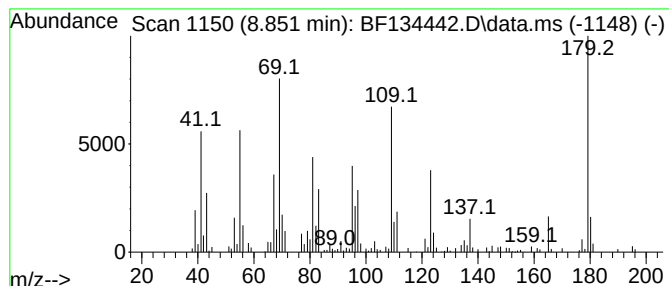
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Peak Number 5 unknown8.851 Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 8.851 | 6.64 ng | 119776 | Naphthalene-d8   | 8.110 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 1,5,9-Decatriene, 2,3,5,8-tetram... | 192 | C14H24       | 230646-72-7  | 27      |      |      |
| 2    | Oxiranecarboxaldehyde, 3-methyl-... | 168 | C10H16O2     | 016996-12-6  | 27      |      |      |
| 3    | 1-Pyrroline, 3-ethyl-               | 97  | C6H11N       | 1000073-06-0 | 22      |      |      |
| 4    | 1-Cyclopentylethanol, chlorodifl... | 226 | C9H13ClF2O2  | 1000376-25-2 | 22      |      |      |
| 5    | Cyclopropane, 1,1-dimethyl-2-(2-... | 124 | C9H16        | 069147-03-1  | 18      |      |      |



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ClientSampleId :  
N48909

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF072423.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 |
| 1,3,6-Trimethyl... | 8.569 | 6.1     | ng    | 110454   | 2                     | 8.110 | 360616 | 20.0 |
| unknown8.651       | 8.651 | 5.8     | ng    | 104215   | 2                     | 8.110 | 360616 | 20.0 |
| unknown8.733       | 8.733 | 8.2     | ng    | 148322   | 2                     | 8.110 | 360616 | 20.0 |
| unknown8.798       | 8.798 | 8.5     | ng    | 153342   | 2                     | 8.110 | 360616 | 20.0 |
| unknown8.851       | 8.851 | 6.6     | ng    | 119776   | 2                     | 8.110 | 360616 | 20.0 |