

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF120817\  
 Data File : BF101241.D  
 Acq On : 8 Dec 2017 17:44  
 Operator : SJ/JU  
 Sample : I6680-09 10X  
 Misc :  
 ALS Vial : 8 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 CL-01-120617-E

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:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.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         | 5.434       | 566           | 569         | 580          | rBB      | 63953          | 68299         | 20.55%          | 2.617%        |
| 2         | 6.451       | 739           | 742         | 756          | rVB      | 68466          | 72572         | 21.84%          | 2.781%        |
| 3         | 6.592       | 763           | 766         | 770          | rBV      | 99419          | 77807         | 23.41%          | 2.982%        |
| 4         | 6.822       | 802           | 805         | 813          | rBB      | 311417         | 241149        | 72.56%          | 9.241%        |
| 5         | 6.975       | 828           | 831         | 837          | rBB      | 67221          | 60955         | 18.34%          | 2.336%        |
| 6         | 7.387       | 898           | 901         | 909          | rBB      | 49043          | 43006         | 12.94%          | 1.648%        |
| 7         | 8.104       | 1019          | 1023        | 1031         | rBV      | 401525         | 320630        | 96.48%          | 12.287%       |
| 8         | 9.175       | 1202          | 1205        | 1209         | rBV      | 109209         | 92166         | 27.73%          | 3.532%        |
| 9         | 9.575       | 1270          | 1273        | 1277         | rBB      | 7010           | 5163          | 1.55%           | 0.198%        |
| 10        | 9.781       | 1306          | 1308        | 1313         | rBB2     | 4230           | 4015          | 1.21%           | 0.154%        |
| 11        | 9.863       | 1318          | 1322        | 1326         | rBV      | 411131         | 332336        | 100.00%         | 12.735%       |
| 12        | 10.651      | 1453          | 1456        | 1461         | rVB      | 48631          | 37286         | 11.22%          | 1.429%        |
| 13        | 10.757      | 1470          | 1474        | 1479         | rBV3     | 4014           | 6405          | 1.93%           | 0.245%        |
| 14        | 11.351      | 1571          | 1575        | 1578         | rBV      | 394110         | 303798        | 91.41%          | 11.642%       |
| 15        | 11.869      | 1658          | 1663        | 1664         | rBV2     | 4232           | 4313          | 1.30%           | 0.165%        |
| 16        | 12.033      | 1688          | 1691        | 1696         | rVB2     | 2691           | 4080          | 1.23%           | 0.156%        |
| 17        | 12.569      | 1779          | 1782        | 1787         | rBV4     | 4027           | 6863          | 2.07%           | 0.263%        |
| 18        | 12.798      | 1818          | 1821        | 1824         | rBV2     | 6895           | 5639          | 1.70%           | 0.216%        |
| 19        | 12.933      | 1840          | 1844        | 1847         | rBV      | 96835          | 80597         | 24.25%          | 3.089%        |
| 20        | 13.116      | 1869          | 1875        | 1879         | rBV6     | 8124           | 14409         | 4.34%           | 0.552%        |
| 21        | 13.286      | 1903          | 1904        | 1907         | rBV3     | 4359           | 4121          | 1.24%           | 0.158%        |
| 22        | 13.357      | 1914          | 1916        | 1917         | rBV2     | 7254           | 5737          | 1.73%           | 0.220%        |
| 23        | 13.374      | 1917          | 1919        | 1923         | rVB4     | 7961           | 8569          | 2.58%           | 0.328%        |
| 24        | 13.421      | 1926          | 1927        | 1930         | rBV3     | 5146           | 5234          | 1.57%           | 0.201%        |
| 25        | 13.463      | 1932          | 1934        | 1938         | rBV5     | 6047           | 6284          | 1.89%           | 0.241%        |
| 26        | 13.498      | 1938          | 1940        | 1942         | rBV2     | 7724           | 5489          | 1.65%           | 0.210%        |
| 27        | 13.574      | 1951          | 1953        | 1956         | rVB3     | 7337           | 7048          | 2.12%           | 0.270%        |
| 28        | 13.739      | 1978          | 1981        | 1985         | rBV5     | 7678           | 13807         | 4.15%           | 0.529%        |
| 29        | 13.821      | 1992          | 1995        | 1998         | rBV5     | 17592          | 18640         | 5.61%           | 0.714%        |
| 30        | 13.851      | 1998          | 2000        | 2003         | rBV4     | 10683          | 12492         | 3.76%           | 0.479%        |
| 31        | 13.998      | 2021          | 2025        | 2029         | rBV      | 344156         | 299733        | 90.19%          | 11.486%       |
| 32        | 15.468      | 2270          | 2275        | 2279         | rBV      | 228978         | 278317        | 83.75%          | 10.665%       |
| 33        | 16.139      | 2386          | 2389        | 2397         | rVB5     | 46954          | 91083         | 27.41%          | 3.490%        |
| 34        | 17.139      | 2557          | 2559        | 2565         | rVB6     | 25634          | 37216         | 11.20%          | 1.426%        |

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ClientSampleId :  
CL-01-120617-E

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:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |       |       |        |        |
|----|--------|------|------|------|------|-------|-------|--------|--------|
| 35 | 17.651 | 2642 | 2646 | 2652 | rBV9 | 12545 | 34303 | 10.32% | 1.315% |
|----|--------|------|------|------|------|-------|-------|--------|--------|

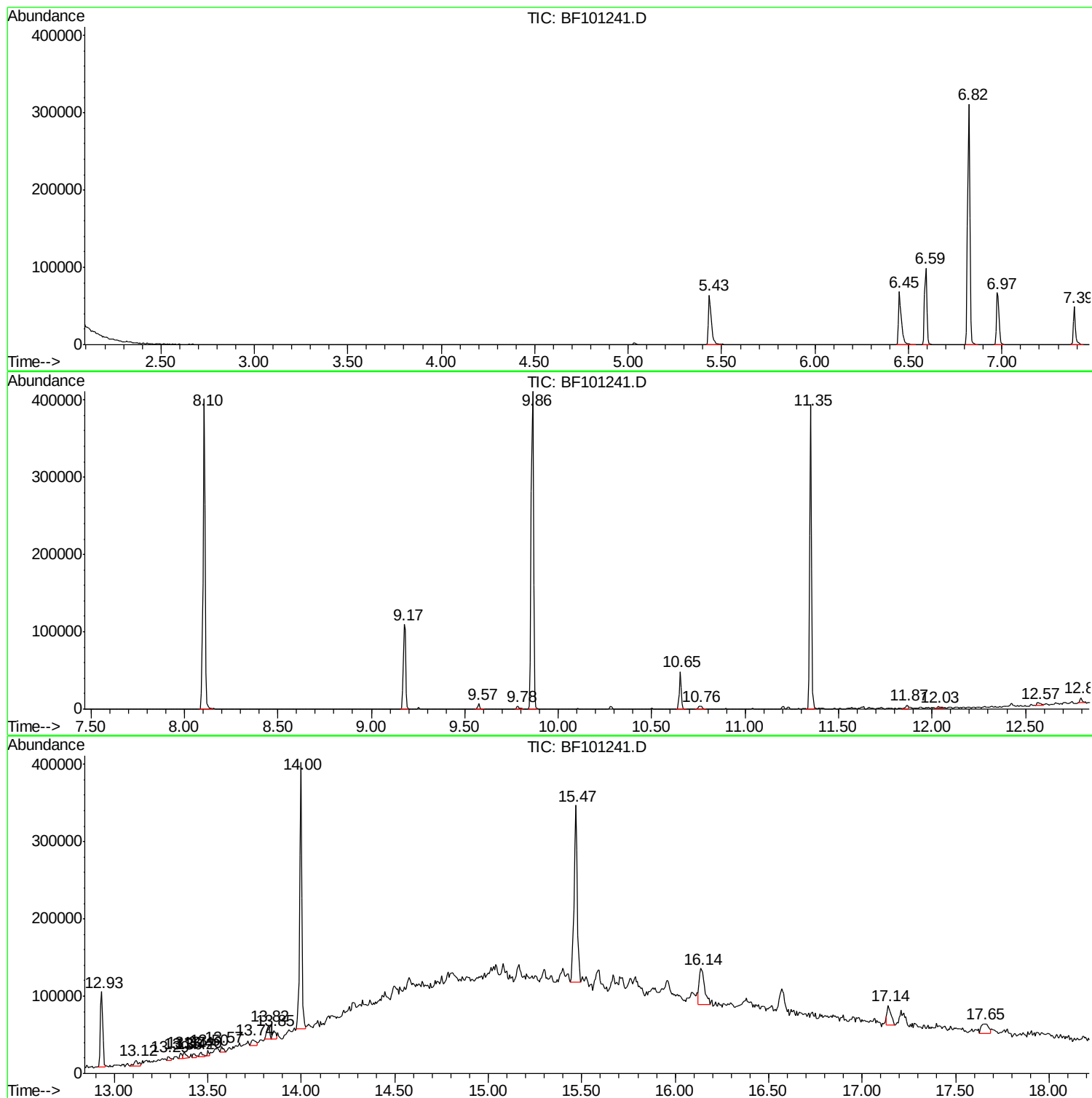
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

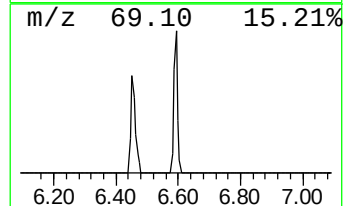
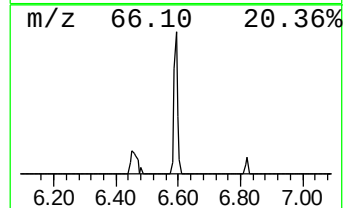
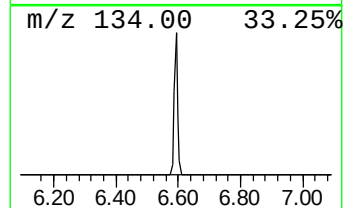
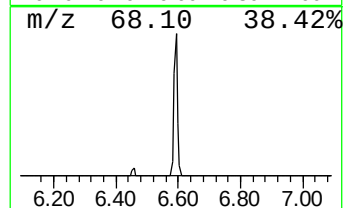
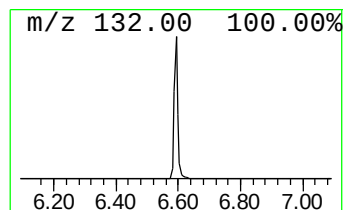
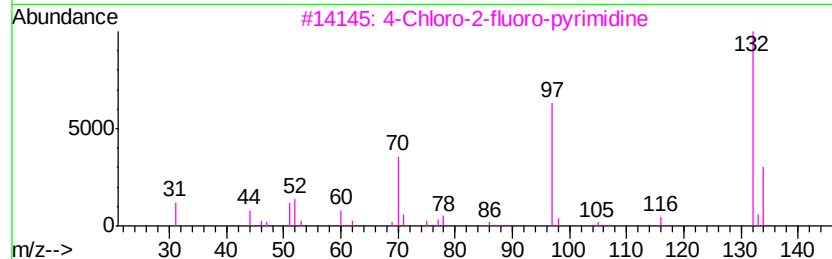
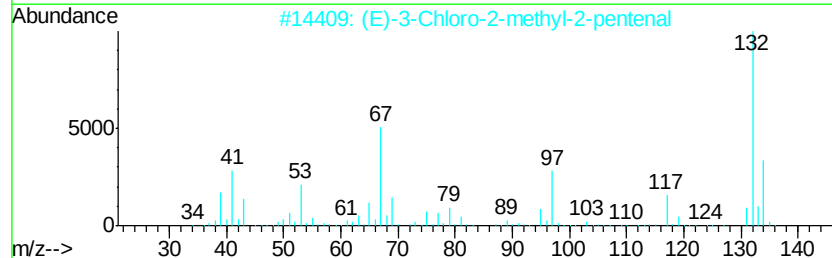
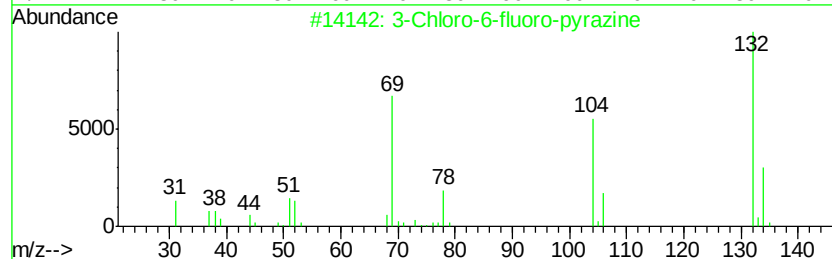
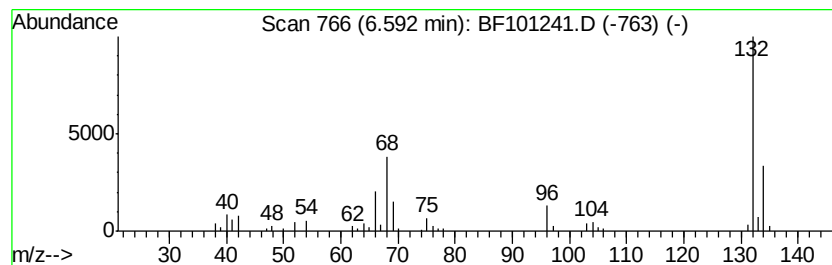
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown6.59 Concentration Rank 2

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 6.59 | 6.45 ng | 77807 | 1,4-Dichlorobenzene-d4 | 6.82 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 12   |
| 4    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 10   |
| 5    |    | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6  | 9    |



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CL-01-120617-E

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

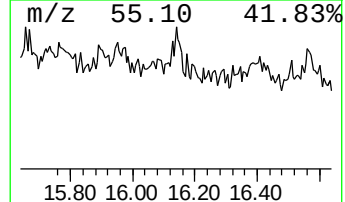
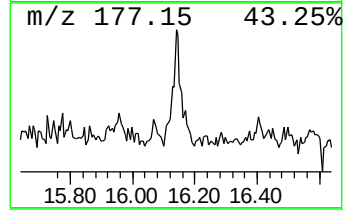
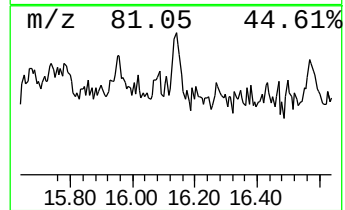
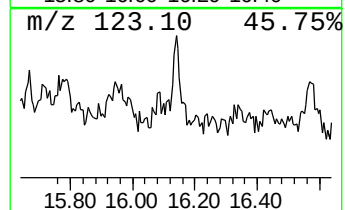
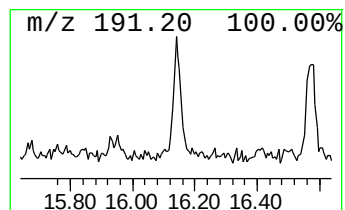
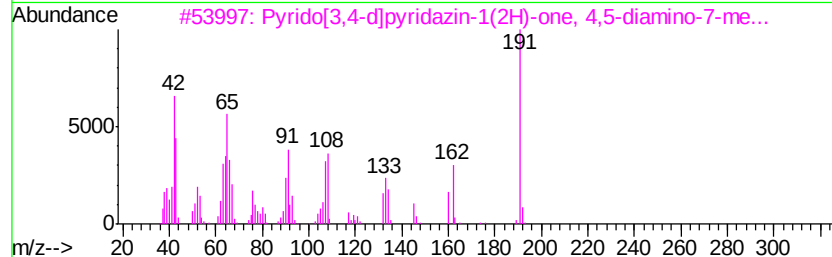
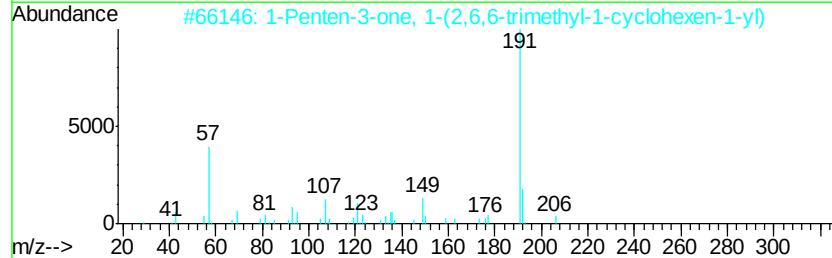
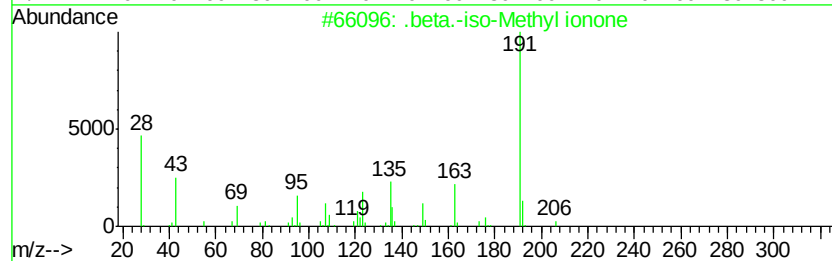
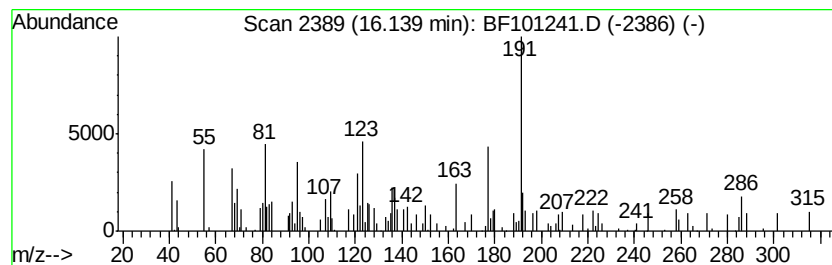
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 unknown16.14 Concentration Rank 1

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 16.14 | 6.55 ng | 91083 | Perylene-d12     | 15.47 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | .beta.-iso-Methyl ionone            | 206 | C14H22O     | 1000285-40-2 | 38   |
| 2    |    | 1-Penten-3-one, 1-(2,6,6-trimeth... | 206 | C14H22O     | 000127-43-5  | 35   |
| 3    |    | Pyrido[3,4-d]pyridazin-1(2H)-one... | 191 | C8H9N5O     | 1000263-69-7 | 30   |
| 4    |    | 3-Indolethanamine, N-acetyl-5-fl... | 250 | C13H15FN2O2 | 1000116-27-1 | 27   |
| 5    |    | N-(4-Morpholin-4-yl-phenyl)-2-ni... | 377 | C17H19N3O5S | 1000374-81-7 | 27   |



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ALS Vial : 8 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF113017.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

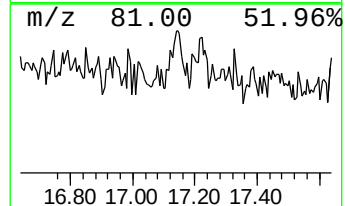
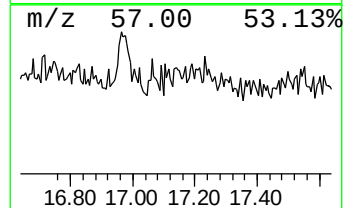
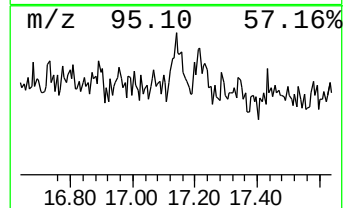
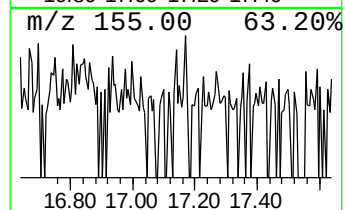
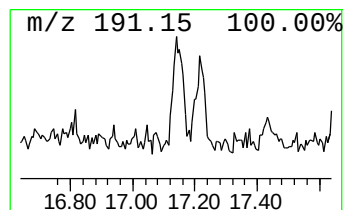
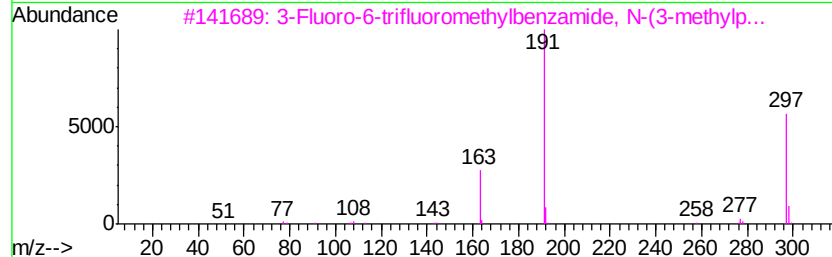
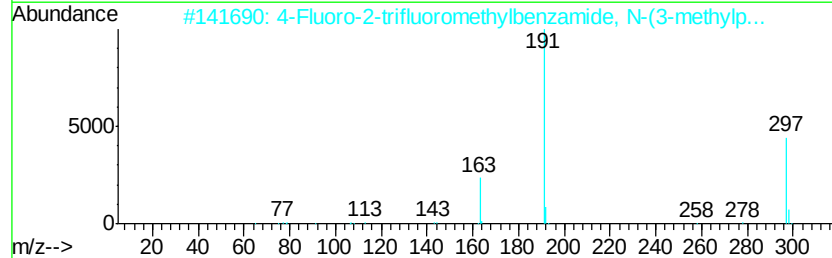
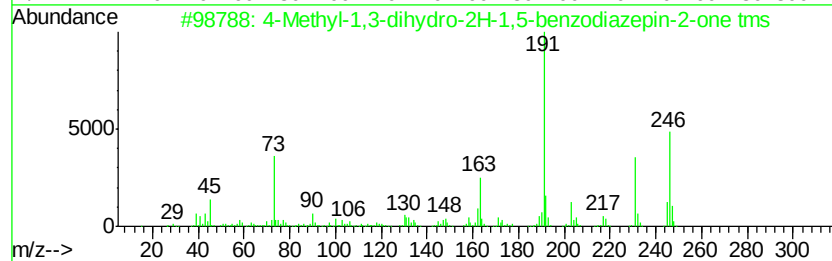
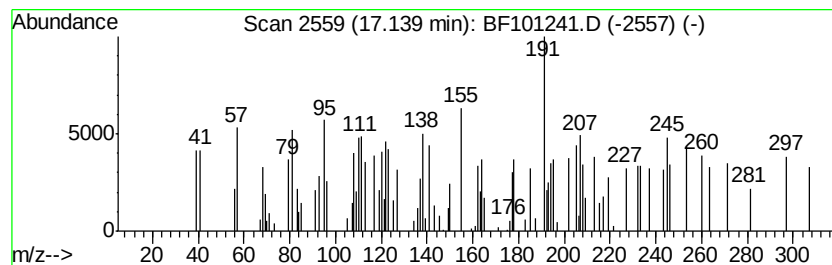
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 unknown17.14 Concentration Rank 4

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 17.14 | 2.67 ng | 37216 | Perylene-d12     | 15.47 |

| Hit# | of                                  | 5   | Tentative ID | MW           | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|--------------|---------|------|------|
| 1    | 4-Methyl-1,3-dihydro-2H-1,5-benz... | 246 | C13H18N2OSi  | 1000331-94-1 | 14      |      |      |
| 2    | 4-Fluoro-2-trifluoromethylbenzam... | 297 | C15H11F4NO   | 1000358-08-9 | 12      |      |      |
| 3    | 3-Fluoro-6-trifluoromethylbenzam... | 297 | C15H11F4NO   | 1000358-07-7 | 12      |      |      |
| 4    | Androstane                          | 260 | C19H32       | 024887-75-0  | 11      |      |      |
| 5    | .beta.-iso-Methyl ionone            | 206 | C14H22O      | 1000285-40-2 | 10      |      |      |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF113017.M  
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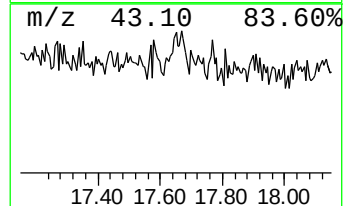
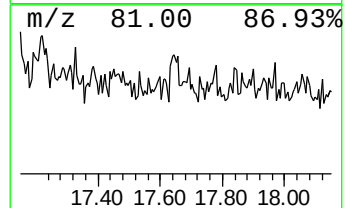
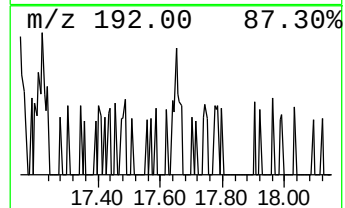
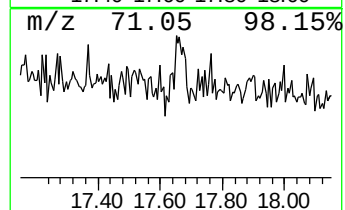
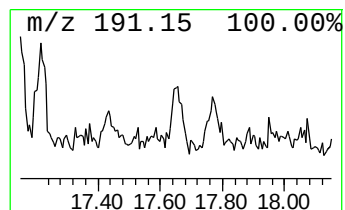
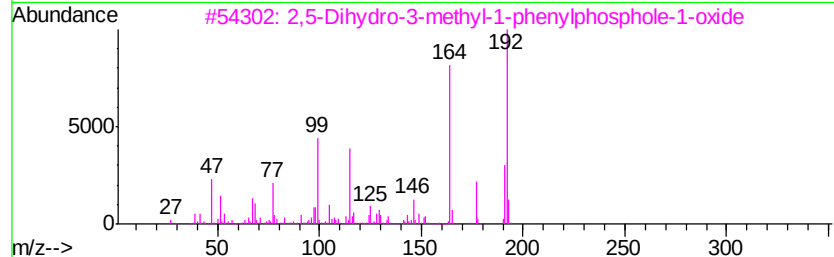
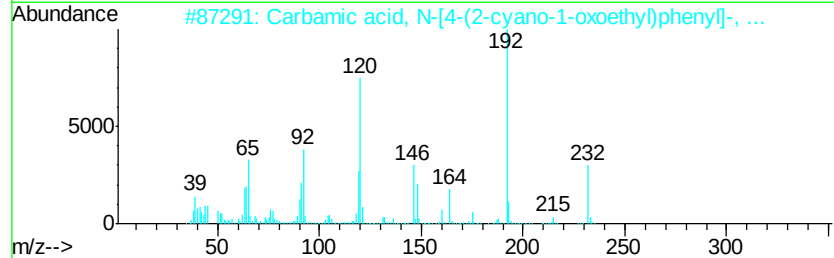
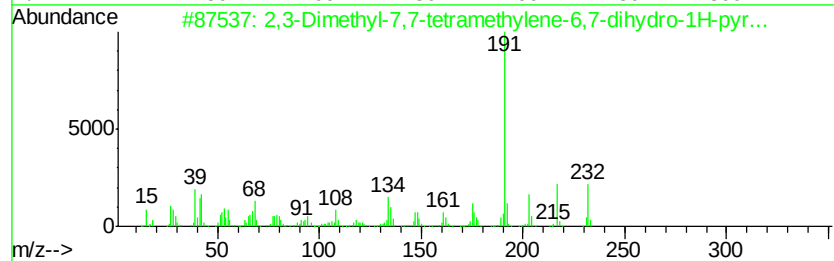
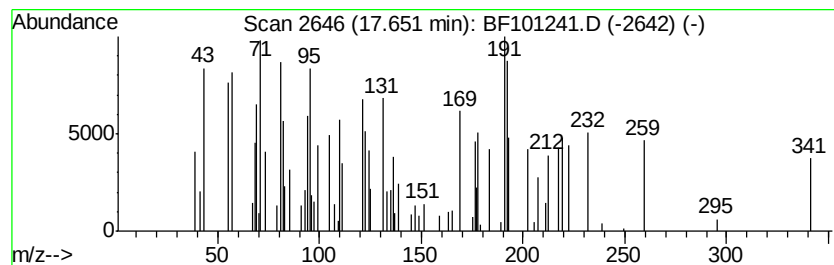
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown17.65 Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 17.65 | 2.47 ng | 34303 | Perylene-d12     | 15.47 |

| Hit# | of                                  | Tentative ID | MW         | MolForm      | CAS# | Qual |
|------|-------------------------------------|--------------|------------|--------------|------|------|
| 1    | 2,3-Dimethyl-7,7-tetramethylene-... | 232          | C13H16N2O2 | 1000287-32-6 | 14   |      |
| 2    | Carbamic acid, N-[4-(2-cyano-1-o... | 232          | C12H12N2O3 | 1000272-00-6 | 11   |      |
| 3    | 2,5-Dihydro-3-methyl-1-phenylpho... | 192          | C11H13OP   | 007564-51-4  | 10   |      |
| 4    | 2-Hydroxy-4-methyl-6-(2-thienyl)... | 192          | C9H8N2OS   | 026963-45-1  | 10   |      |
| 5    | Cycloheptene, 1-iodo-               | 222          | C7H11I     | 049565-03-9  | 10   |      |



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

| TIC Top Hit name | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                  |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown6.59      | 6.59  | 6.5     | ng    | 77807    | 1                     | 6.82  | 241149 | 20.0 |
| unknown16.14     | 16.14 | 6.5     | ng    | 91083    | 6                     | 15.47 | 278317 | 20.0 |
| unknown17.14     | 17.14 | 2.7     | ng    | 37216    | 6                     | 15.47 | 278317 | 20.0 |
| unknown17.65     | 17.65 | 2.5     | ng    | 34303    | 6                     | 15.47 | 278317 | 20.0 |