

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072116\  
 Data File : BF089185.D  
 Acq On : 21 Jul 2016 17:43  
 Operator : UM/SJ  
 Sample : H4129-03 10X  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 KSB-10-0.2-2.0

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-BF072016.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         | 1.724       | 10            | 12          | 47           | rVB      | 720354         | 1824519       | 100.00%         | 39.500%       |
| 2         | 5.187       | 312           | 315         | 327          | rBV      | 25134          | 62694         | 3.44%           | 1.357%        |
| 3         | 6.262       | 407           | 409         | 417          | rBV      | 34167          | 77852         | 4.27%           | 1.685%        |
| 4         | 6.365       | 417           | 418         | 424          | rVV      | 60487          | 85265         | 4.67%           | 1.846%        |
| 5         | 6.593       | 436           | 438         | 450          | rBV      | 176674         | 268001        | 14.69%          | 5.802%        |
| 6         | 6.753       | 450           | 452         | 461          | rVB      | 73168          | 73690         | 4.04%           | 1.595%        |
| 7         | 7.165       | 487           | 488         | 500          | rBB      | 34705          | 53238         | 2.92%           | 1.153%        |
| 8         | 7.885       | 549           | 551         | 564          | rBV      | 371009         | 352599        | 19.33%          | 7.634%        |
| 9         | 8.959       | 643           | 645         | 652          | rBV      | 112404         | 102455        | 5.62%           | 2.218%        |
| 10        | 9.633       | 701           | 704         | 706          | rBV      | 261505         | 312205        | 17.11%          | 6.759%        |
| 11        | 10.411      | 770           | 772         | 775          | rBB      | 27654          | 27518         | 1.51%           | 0.596%        |
| 12        | 11.096      | 830           | 832         | 835          | rBV      | 184878         | 260169        | 14.26%          | 5.633%        |
| 13        | 12.308      | 936           | 938         | 941          | rVB      | 20231          | 23258         | 1.27%           | 0.504%        |
| 14        | 12.525      | 955           | 957         | 962          | rVV      | 22872          | 39523         | 2.17%           | 0.856%        |
| 15        | 12.685      | 969           | 971         | 973          | rBV      | 71927          | 92288         | 5.06%           | 1.998%        |
| 16        | 12.857      | 982           | 986         | 988          | rBV2     | 14679          | 27433         | 1.50%           | 0.594%        |
| 17        | 12.971      | 994           | 996         | 1000         | rBV4     | 10008          | 29453         | 1.61%           | 0.638%        |
| 18        | 13.177      | 1011          | 1014        | 1017         | rBV4     | 8773           | 25606         | 1.40%           | 0.554%        |
| 19        | 13.725      | 1059          | 1062        | 1066         | rBV      | 298451         | 367170        | 20.12%          | 7.949%        |
| 20        | 15.074      | 1178          | 1180        | 1184         | rBV      | 192543         | 238624        | 13.08%          | 5.166%        |
| 21        | 15.657      | 1228          | 1231        | 1236         | rVB2     | 52751          | 117798        | 6.46%           | 2.550%        |
| 22        | 16.011      | 1260          | 1262        | 1271         | rVB      | 42387          | 87940         | 4.82%           | 1.904%        |
| 23        | 16.548      | 1307          | 1309        | 1317         | rVB4     | 30554          | 69693         | 3.82%           | 1.509%        |

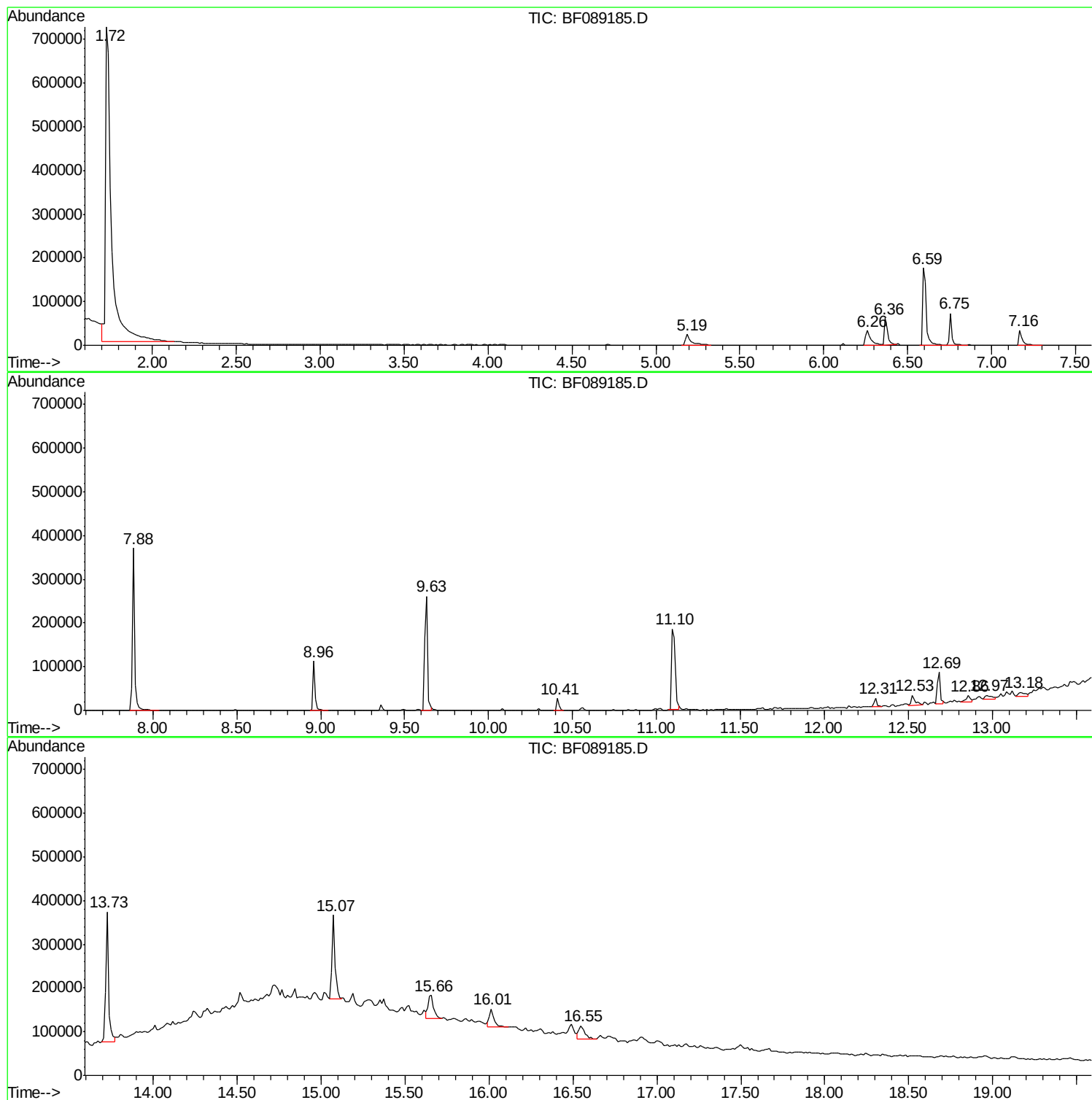
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ClientSampleId :  
KSB-10-0.2-2.0

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072016.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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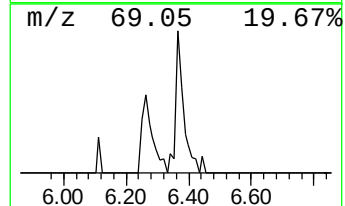
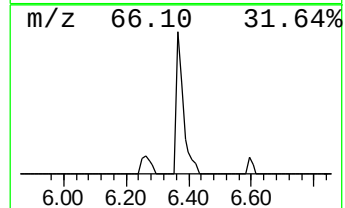
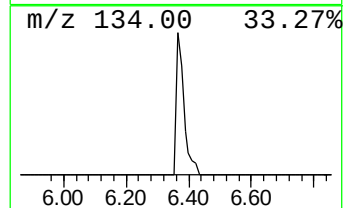
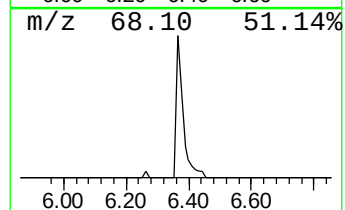
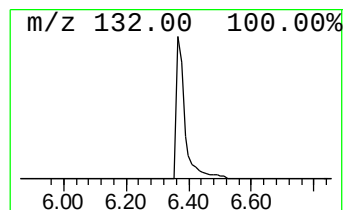
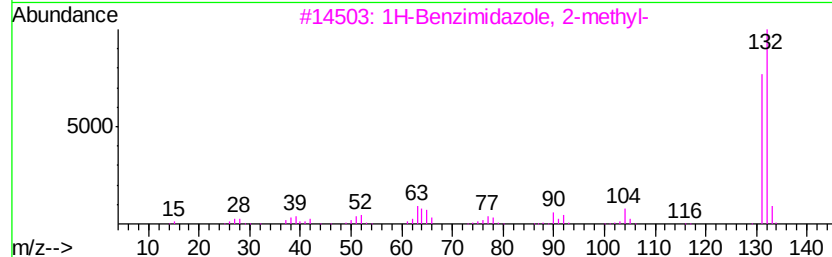
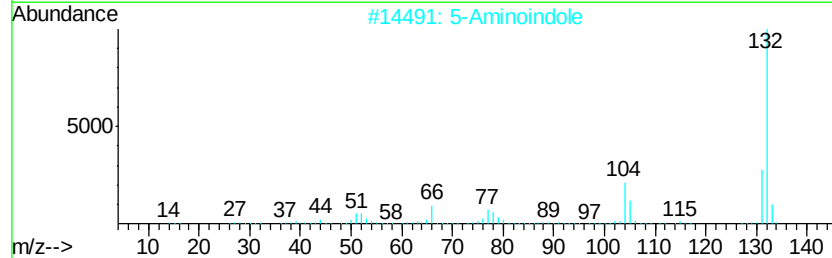
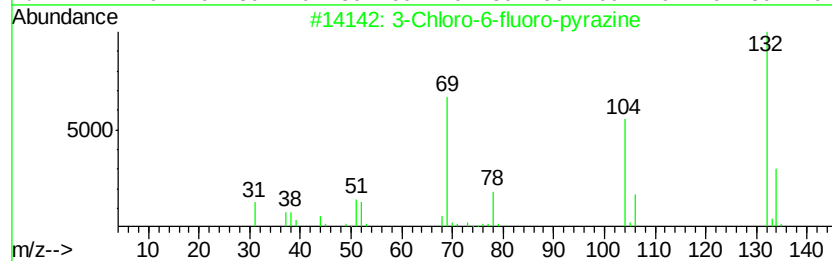
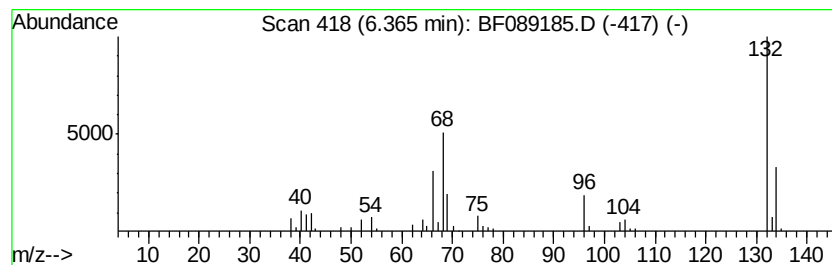
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.36 Concentration Rank 4

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 6.36 | 6.36 ng | 85265 | 1,4-Dichlorobenzene-d4 | 6.60 |

| Hit# | of                   | Tentative ID              | MW  | MolForm   | CAS#         | Qual |
|------|----------------------|---------------------------|-----|-----------|--------------|------|
| 1    | 3                    | Chloro-6-fluoro-pyrazine  | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    | 5                    | Aminoindole               | 132 | C8H8N2    | 005192-03-0  | 22   |
| 3    | 1H                   | Benzimidazole, 2-methyl-  | 132 | C8H8N2    | 000615-15-6  | 22   |
| 4    | 5                    | Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0  | 12   |
| 5    | (5-Methyl-2-pyridyl) | acetonitrile              | 132 | C8H8N2    | 1000241-93-9 | 10   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

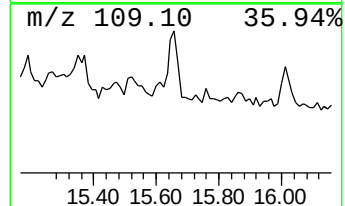
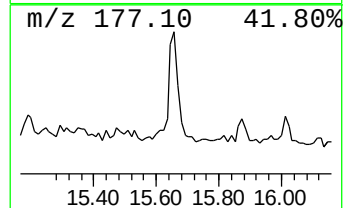
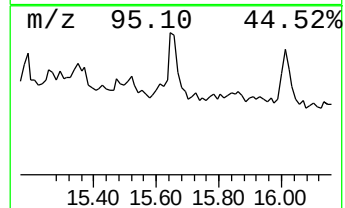
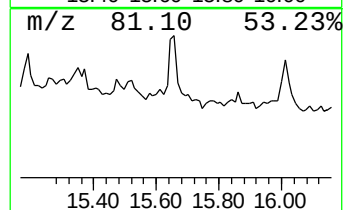
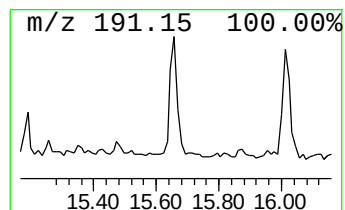
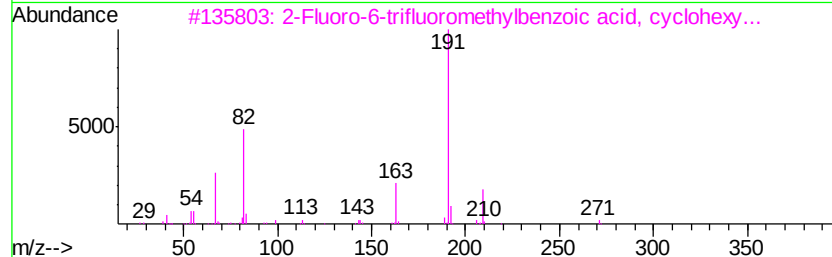
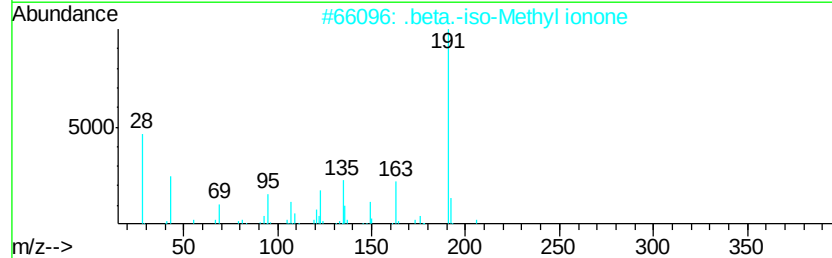
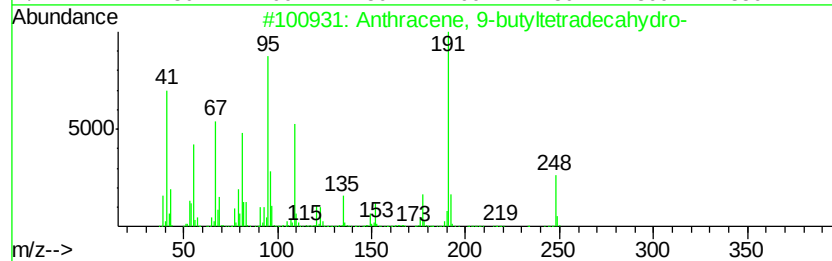
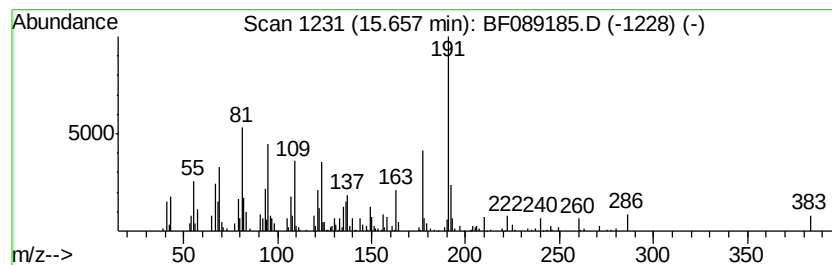
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 unknown15.66 Concentration Rank 2

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.66 | 9.87 ng | 117798 | Perylene-d12     | 15.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | Anthracene, 9-butyltetradecahydro-  | 248 | C18H32     | 055133-89-6  | 40   |
| 2    |    | .beta.-iso-Methyl ionone            | 206 | C14H22O    | 1000285-40-2 | 38   |
| 3    |    | 2-Fluoro-6-trifluoromethylbenzoi... | 290 | C14H14F4O2 | 1000357-69-3 | 27   |
| 4    |    | 2-Imino-3-phenyl-4-thiazolidinone   | 192 | C9H8N2OS   | 006966-55-8  | 27   |
| 5    |    | 2,4,7-Pteridinetriamine, 6-methyl-  | 191 | C7H9N7     | 017539-50-3  | 27   |



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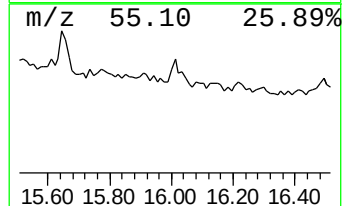
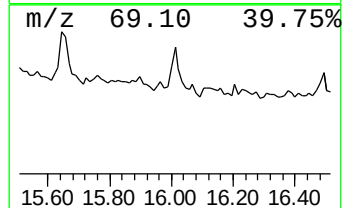
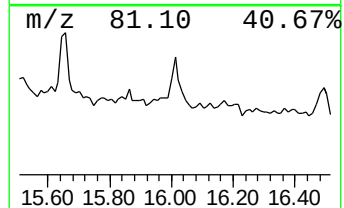
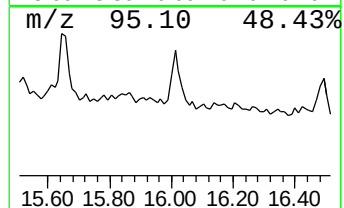
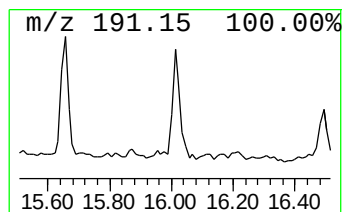
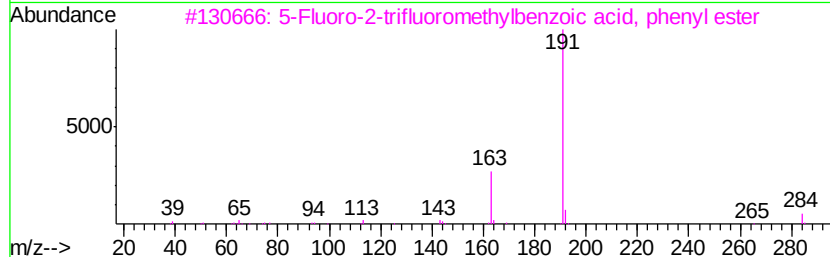
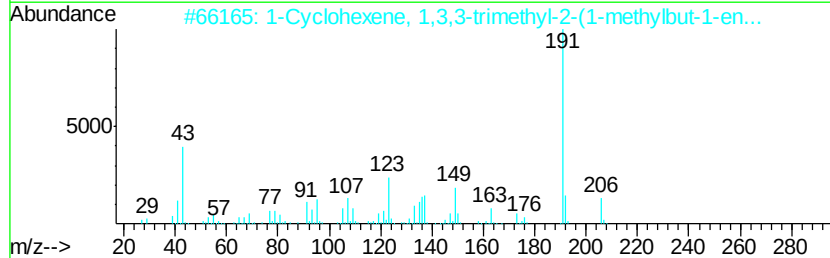
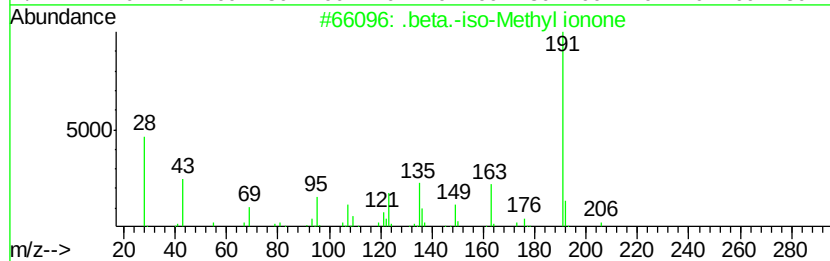
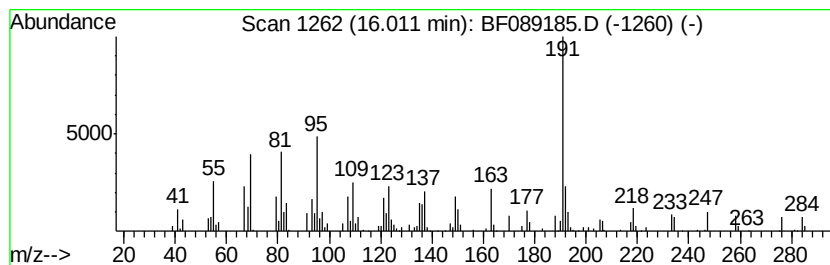
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 .beta.-iso-Methyl ionone Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 16.01 | 7.37 ng | 87940 | Perylene-d12     | 15.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | .beta.-iso-Methyl ionone            | 206 | C14H22O   | 1000285-40-2 | 64   |
| 2    |    | 1-Cyclohexene, 1,3,3-trimethyl-2... | 206 | C14H22O   | 1000197-08-4 | 38   |
| 3    |    | 5-Fluoro-2-trifluoromethylbenzoi... | 284 | C14H8F4O2 | 1000357-62-7 | 35   |
| 4    |    | 3-Fluoro-4-trifluoromethylbenzoi... | 284 | C14H8F4O2 | 1000357-93-7 | 35   |
| 5    |    | Anthracene, 9-butyltetradecahydro-  | 248 | C18H32    | 055133-89-6  | 35   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072016.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

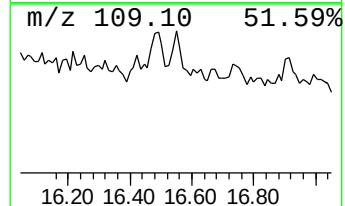
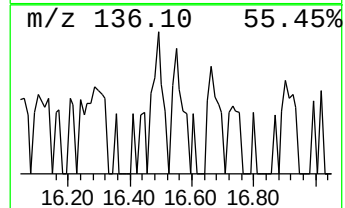
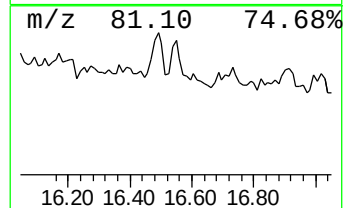
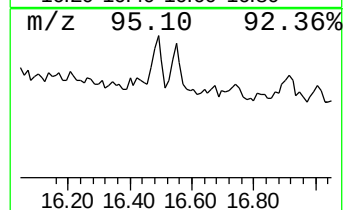
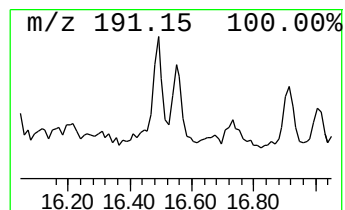
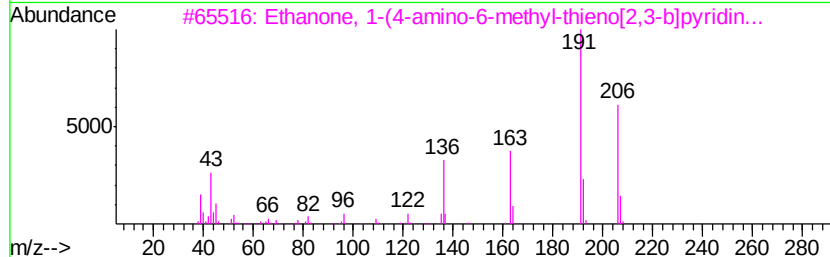
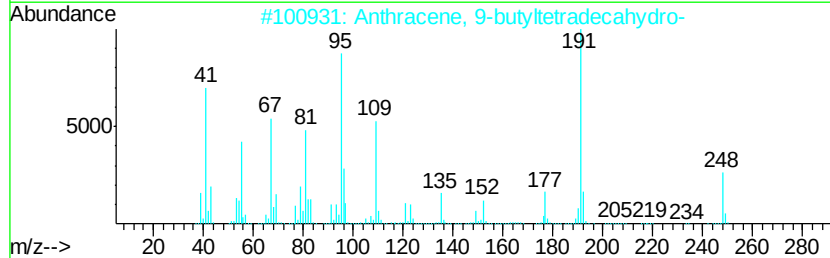
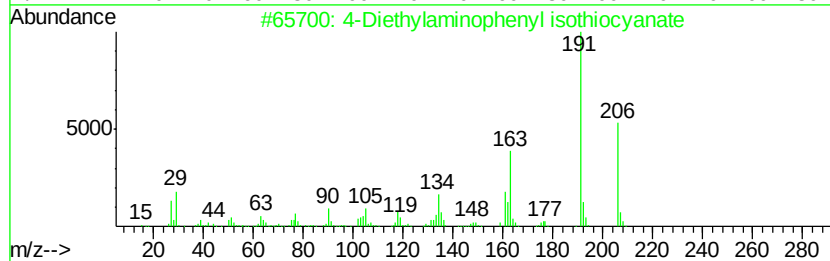
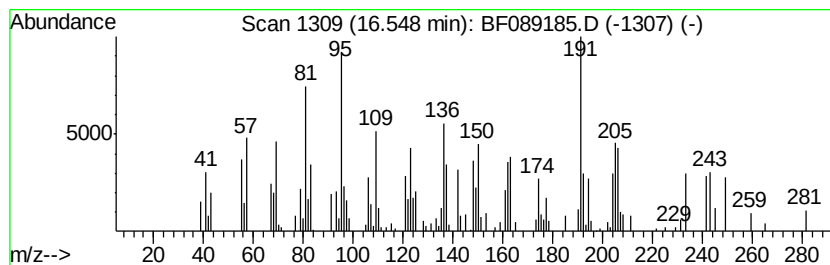
TIC Library : C:\Database\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 unknown16.55 Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 16.55 | 5.84 ng | 69693 | Perylene-d12     | 15.07 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | 4-Diethylaminophenyl isothiocyanate | 206 | C11H14N2S  | 084381-54-4  | 38   |
| 2    |    | Anthracene, 9-butyltetradecahydro-  | 248 | C18H32     | 055133-89-6  | 30   |
| 3    |    | Ethanone, 1-(4-amino-6-methyl-th... | 206 | C10H10N2OS | 1000268-83-5 | 27   |
| 4    |    | 2-Furoic acid, 2-methyloct-5-yn-... | 234 | C14H18O3   | 1000299-23-7 | 27   |
| 5    |    | 2,5,5,8a-Tetramethyl-4-methylene... | 206 | C14H22O    | 093175-76-9  | 25   |



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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 |
| unknown6.36          | 6.36  | 6.4     | ng    | 85265    | 1                     | 6.60  | 268001 | 20.0 |
| unknown15.66         | 15.66 | 9.9     | ng    | 117798   | 6                     | 15.07 | 238624 | 20.0 |
| .beta.-iso-Methyl... | 16.01 | 7.4     | ng    | 87940    | 6                     | 15.07 | 238624 | 20.0 |
| unknown16.55         | 16.55 | 5.8     | ng    | 69693    | 6                     | 15.07 | 238624 | 20.0 |