

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF122916\  
 Data File : BF092031.D  
 Acq On : 29 Dec 2016 18:34  
 Operator : UM/SJ  
 Sample : H6301-02  
 Misc :  
 ALS Vial : 17 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 MW-12

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-BF122116.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         | 4.830       | 238           | 240         | 248          | rBV      | 641927         | 769432        | 10.53%          | 1.369%        |
| 2         | 5.299       | 278           | 281         | 283          | rBV      | 2777965        | 2855802       | 39.07%          | 5.082%        |
| 3         | 6.350       | 371           | 373         | 375          | rBV      | 2234500        | 2079898       | 28.46%          | 3.701%        |
| 4         | 6.465       | 380           | 383         | 385          | rBV      | 5411792        | 4987271       | 68.24%          | 8.875%        |
| 5         | 6.693       | 400           | 403         | 405          | rBV      | 1117523        | 1269346       | 17.37%          | 2.259%        |
| 6         | 6.842       | 414           | 416         | 419          | rBV      | 3450917        | 4188306       | 57.30%          | 7.453%        |
| 7         | 7.265       | 450           | 453         | 455          | rBV      | 3107567        | 4049380       | 55.40%          | 7.206%        |
| 8         | 7.973       | 513           | 515         | 518          | rBV      | 1605945        | 1551499       | 21.23%          | 2.761%        |
| 9         | 9.059       | 607           | 610         | 612          | rBV      | 7230188        | 7308828       | 100.00%         | 13.006%       |
| 10        | 9.459       | 642           | 645         | 647          | rBV      | 118662         | 152809        | 2.09%           | 0.272%        |
| 11        | 9.722       | 666           | 668         | 671          | rBV      | 1775886        | 2179949       | 29.83%          | 3.879%        |
| 12        | 10.522      | 735           | 738         | 740          | rBV      | 3854076        | 4714717       | 64.51%          | 8.390%        |
| 13        | 10.648      | 747           | 749         | 753          | rVB      | 54622          | 90891         | 1.24%           | 0.162%        |
| 14        | 11.208      | 795           | 798         | 800          | rBV      | 2543839        | 2255993       | 30.87%          | 4.015%        |
| 15        | 11.756      | 844           | 846         | 850          | rBV2     | 72133          | 128280        | 1.76%           | 0.228%        |
| 16        | 12.797      | 934           | 937         | 940          | rBV      | 6118390        | 7134234       | 97.61%          | 12.695%       |
| 17        | 13.700      | 1013          | 1016        | 1020         | rBV3     | 134416         | 216149        | 2.96%           | 0.385%        |
| 18        | 13.837      | 1026          | 1028        | 1031         | rBV      | 2273912        | 2186129       | 29.91%          | 3.890%        |
| 19        | 14.328      | 1067          | 1071        | 1073         | rBV2     | 86999          | 109648        | 1.50%           | 0.195%        |
| 20        | 14.625      | 1094          | 1097        | 1099         | rBV      | 155379         | 225410        | 3.08%           | 0.401%        |
| 21        | 14.922      | 1120          | 1123        | 1126         | rBV      | 411349         | 448931        | 6.14%           | 0.799%        |
| 22        | 15.220      | 1146          | 1149        | 1151         | rBV      | 1412984        | 1696140       | 23.21%          | 3.018%        |
| 23        | 15.265      | 1151          | 1153        | 1156         | rVB      | 645786         | 819562        | 11.21%          | 1.458%        |
| 24        | 15.643      | 1183          | 1186        | 1190         | rBV      | 571589         | 978019        | 13.38%          | 1.740%        |
| 25        | 16.088      | 1222          | 1225        | 1234         | rVB      | 600947         | 1125463       | 15.40%          | 2.003%        |
| 26        | 16.614      | 1267          | 1271        | 1281         | rBV      | 401706         | 890616        | 12.19%          | 1.585%        |
| 27        | 17.220      | 1319          | 1324        | 1335         | rVB      | 322114         | 824360        | 11.28%          | 1.467%        |
| 28        | 17.940      | 1382          | 1387        | 1394         | rBV      | 172218         | 513769        | 7.03%           | 0.914%        |
| 29        | 18.797      | 1456          | 1462        | 1470         | rBV      | 118441         | 445059        | 6.09%           | 0.792%        |

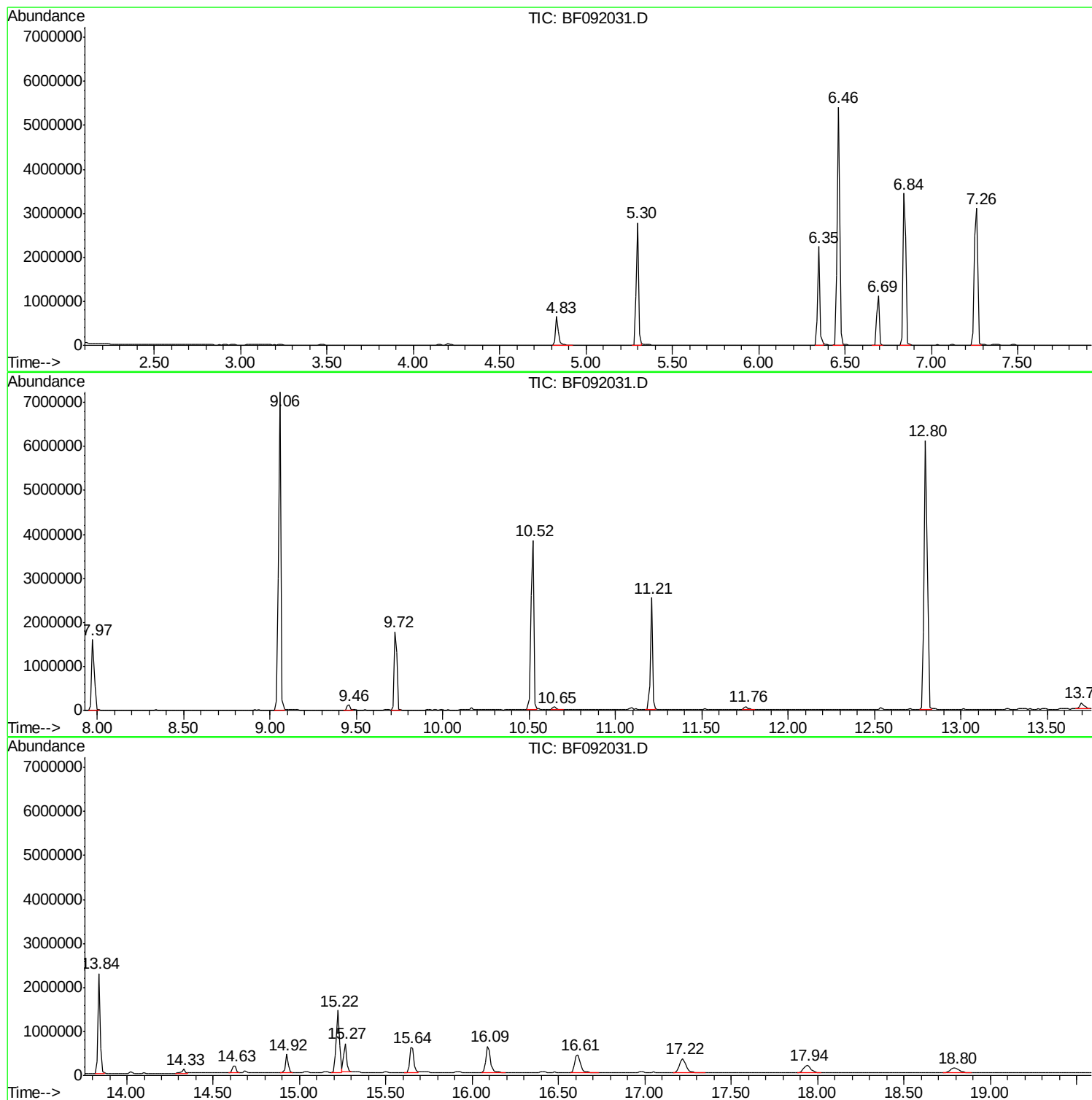
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BNA\_F  
ClientSampleId :  
MW-12

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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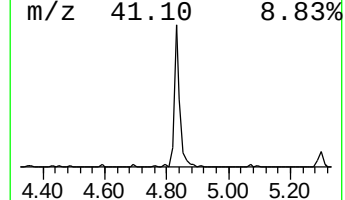
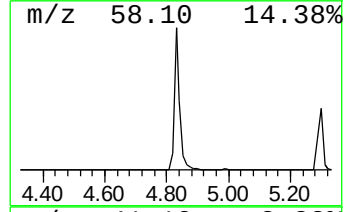
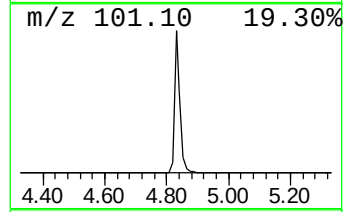
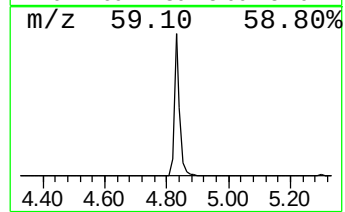
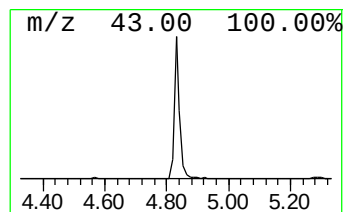
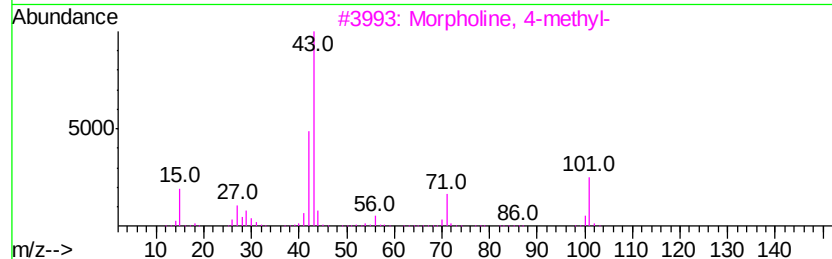
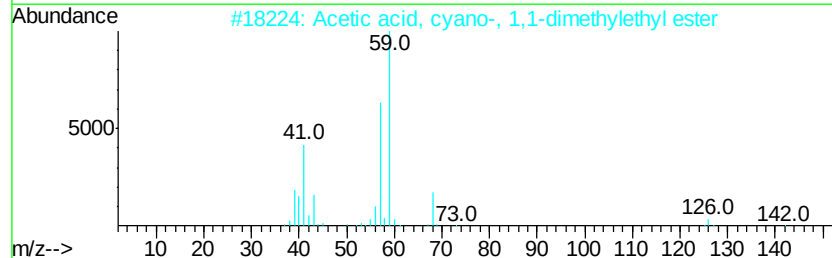
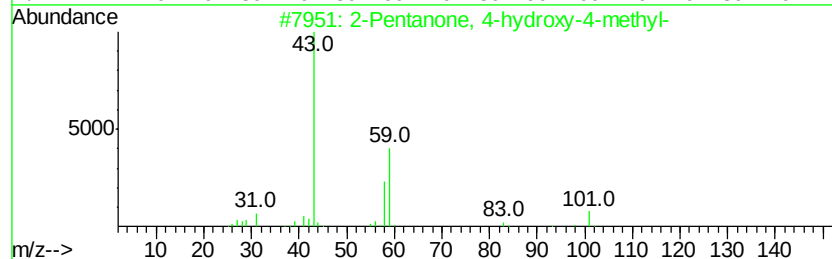
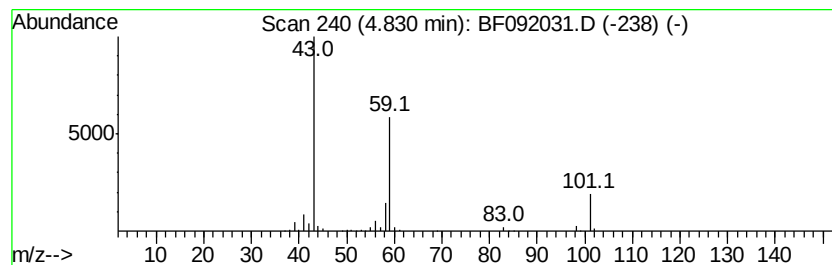
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.83 | 12.12 ng | 769432 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# | of | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|--------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 56   |
| 2    |    | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 3    |    | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |
| 4    |    | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | 4-Hydroxy-3-hexanone                 | 116 | C6H12O2  | 004984-85-4 | 9    |



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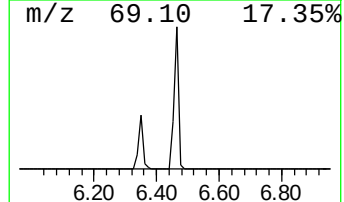
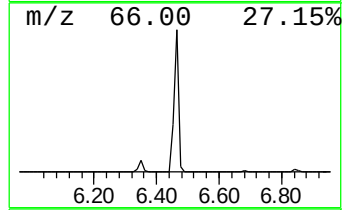
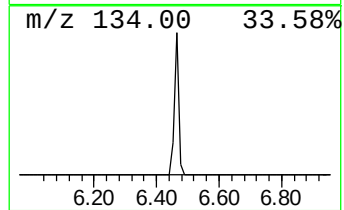
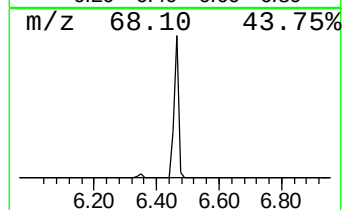
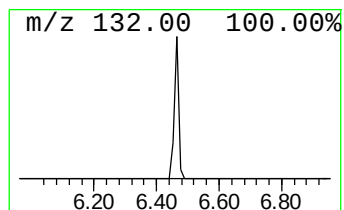
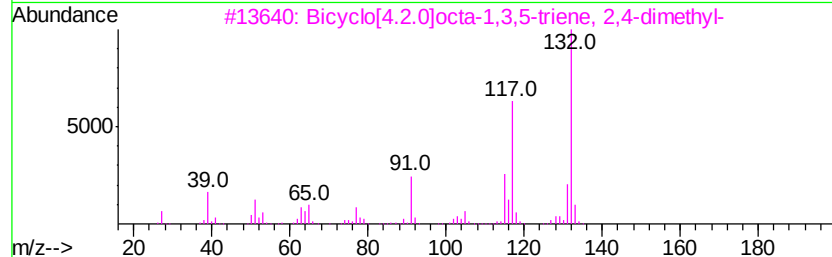
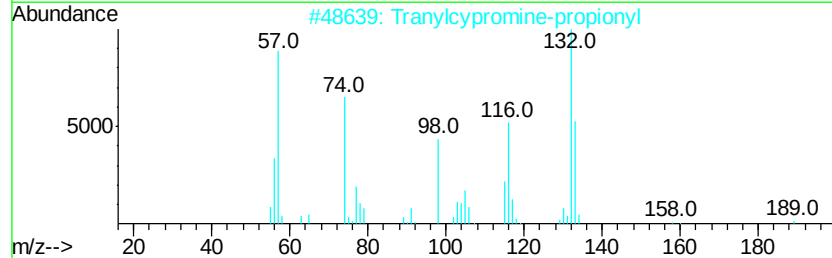
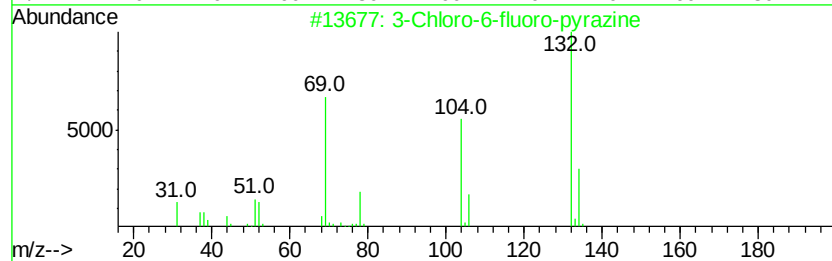
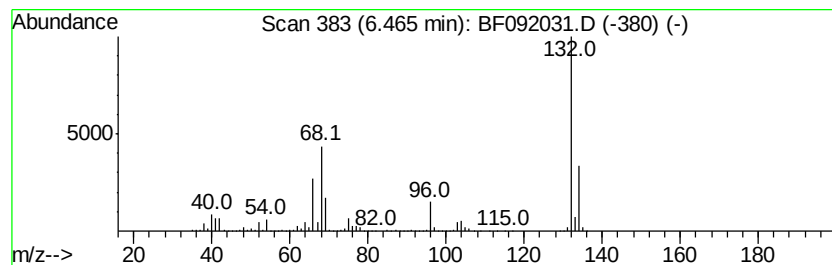
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.46 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.46 | 78.58 ng | 4987270 | 1,4-Dichlorobenzene-d4 | 6.69 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 9    |
| 5    |    | 4-Chloro-2-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-00-5  | 9    |



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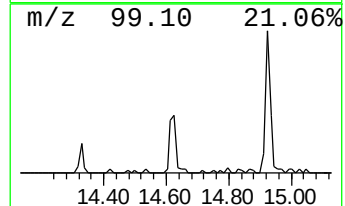
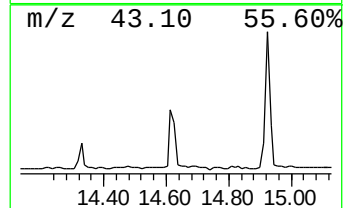
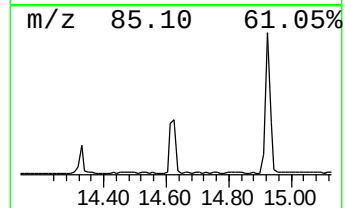
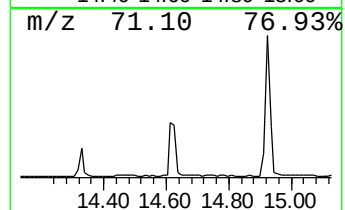
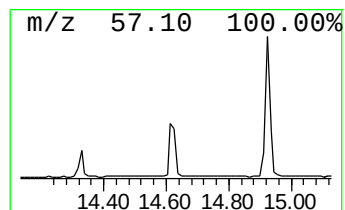
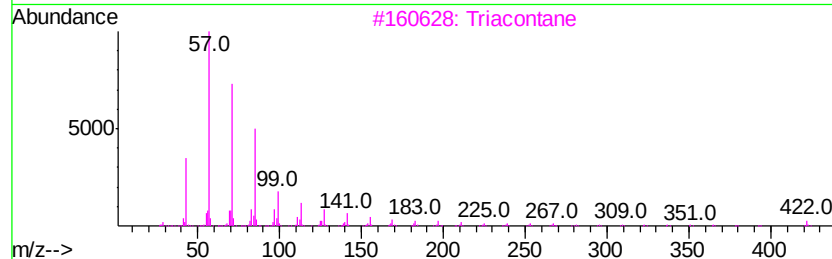
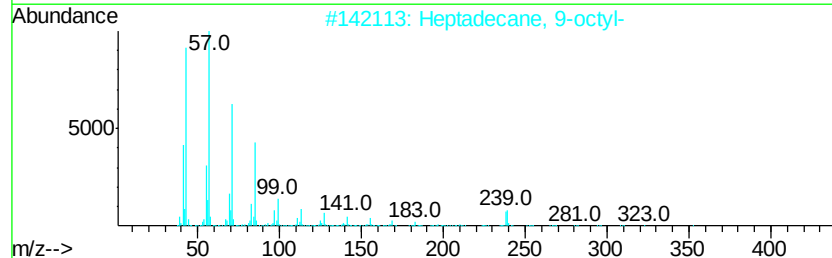
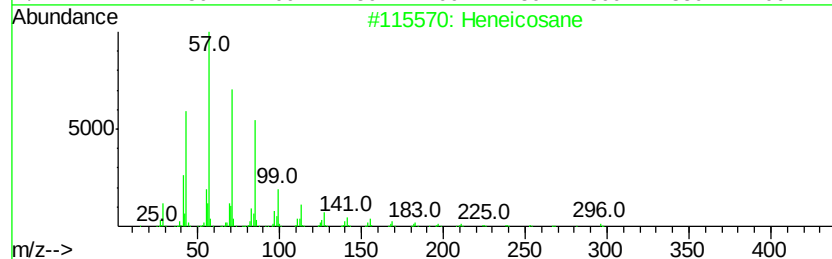
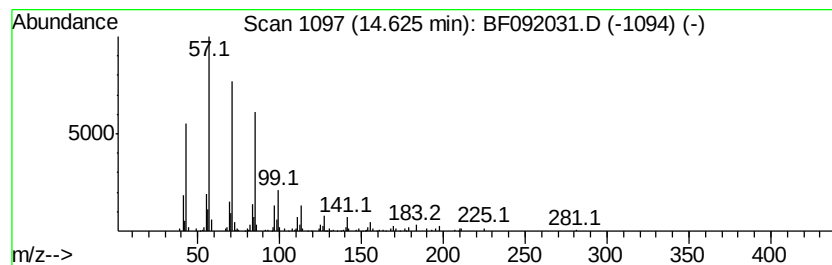
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Heneicosane Concentration Rank 11

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.63 | 2.66 ng | 225410 | Perylene-d12     | 15.22 |

| Hit# of | 5                             | Tentative ID | MW  | MolForm | CAS#         | Qual |
|---------|-------------------------------|--------------|-----|---------|--------------|------|
| 1       | Heneicosane                   |              | 296 | C21H44  | 000629-94-7  | 91   |
| 2       | Heptadecane, 9-octyl-         |              | 352 | C25H52  | 007225-64-1  | 91   |
| 3       | Triacotane                    |              | 422 | C30H62  | 000638-68-6  | 91   |
| 4       | Eicosane, 7-hexyl-            |              | 366 | C26H54  | 055333-99-8  | 90   |
| 5       | Tridecanol, 2-ethyl-2-methyl- |              | 242 | C16H34O | 1000115-66-1 | 90   |



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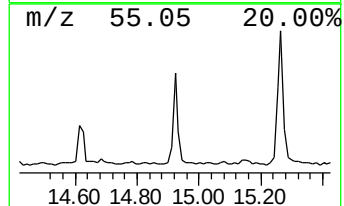
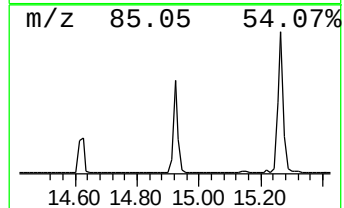
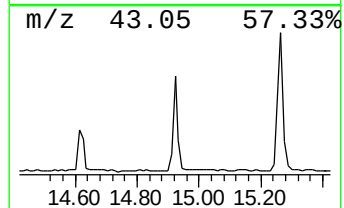
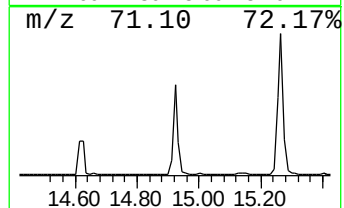
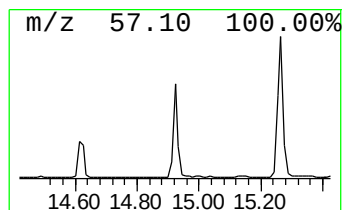
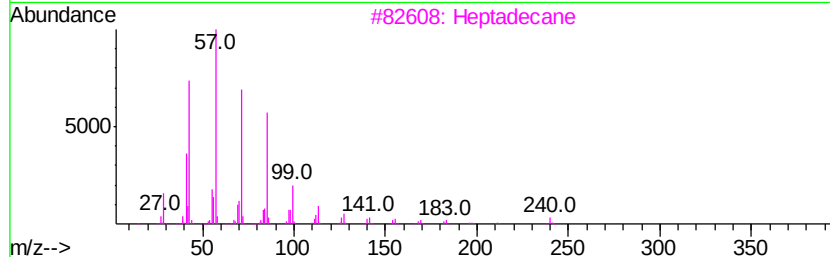
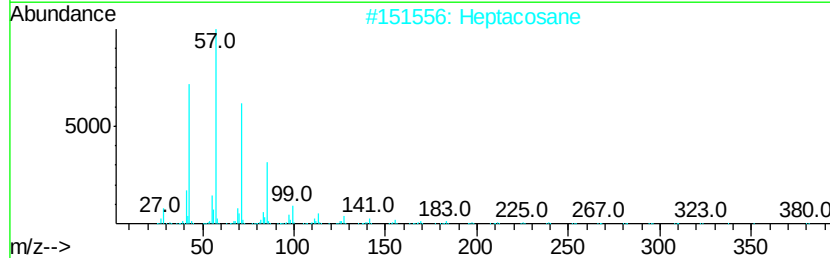
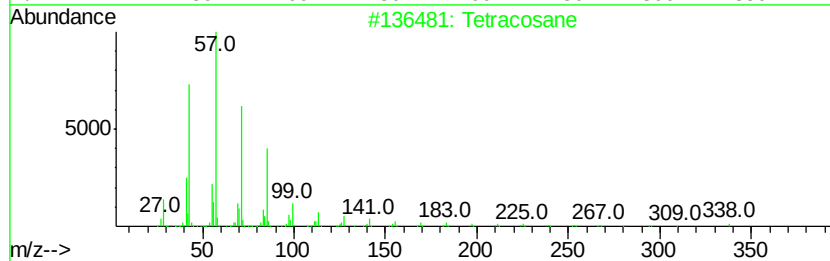
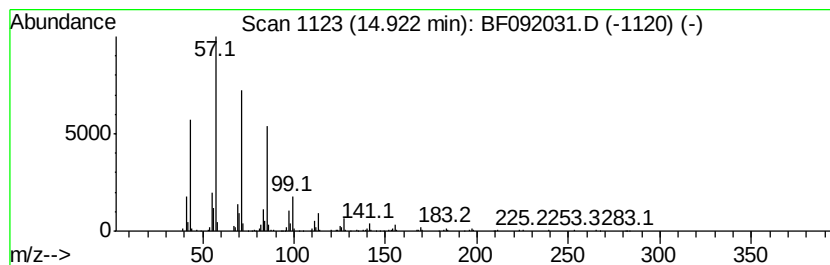
TIC Library : C:\DATABASE\NIST02.L  
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Peak Number 5 Tetracosane Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.92 | 5.29 ng | 448931 | Perylene-d12     | 15.22 |

| Hit# of | 5 | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|---|--------------|-----|---------|-------------|------|
| 1       |   | Tetracosane  | 338 | C24H50  | 000646-31-1 | 90   |
| 2       |   | Heptacosane  | 380 | C27H56  | 000593-49-7 | 87   |
| 3       |   | Heptadecane  | 240 | C17H36  | 000629-78-7 | 86   |
| 4       |   | Heneicosane  | 296 | C21H44  | 000629-94-7 | 86   |
| 5       |   | Octacosane   | 394 | C28H58  | 000630-02-4 | 81   |



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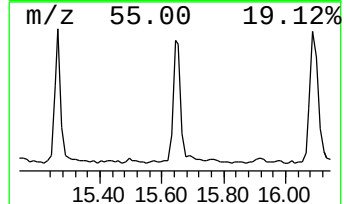
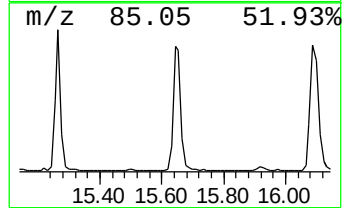
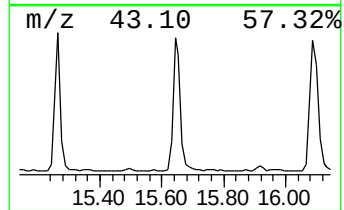
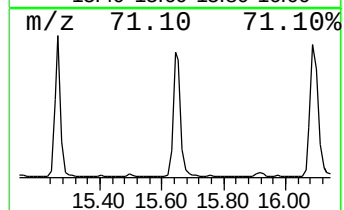
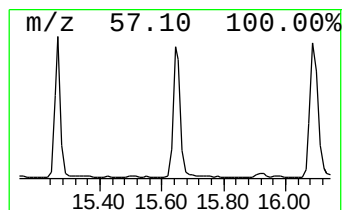
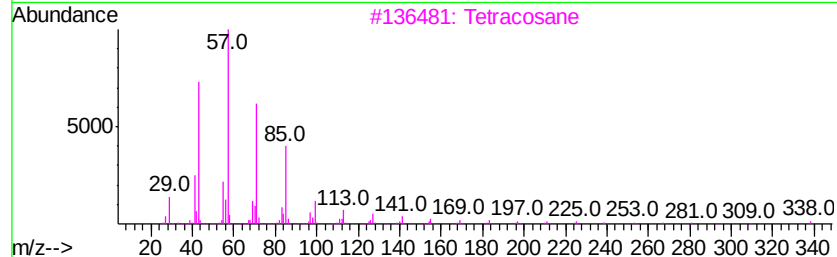
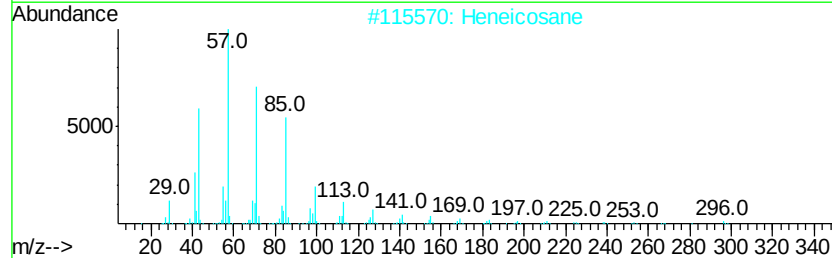
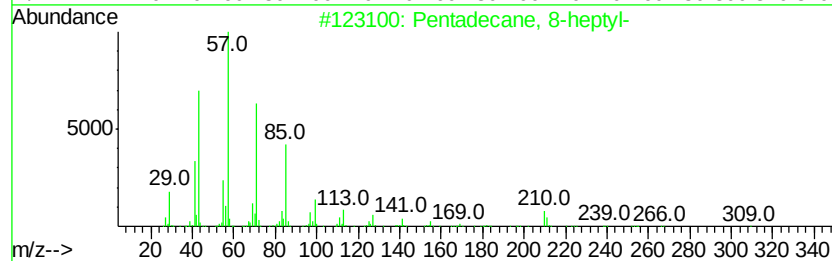
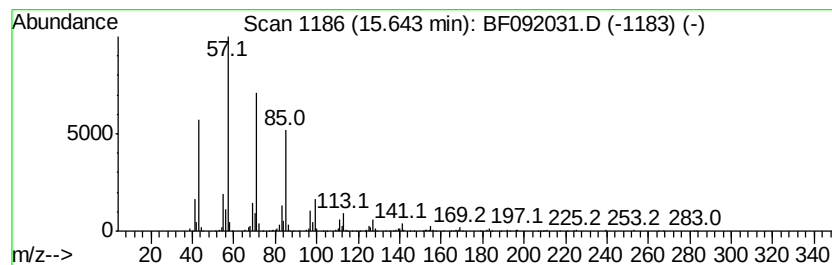
Instrument :  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Pentadecane, 8-heptyl- Concentration Rank 5

| R.T.      | EstConc                | Area   | Relative to ISTD | R.T.        |      |
|-----------|------------------------|--------|------------------|-------------|------|
| 15.64     | 11.53 ng               | 978019 | Perylene-d12     | 15.22       |      |
| Hit# of 5 | Tentative ID           | MW     | MolForm          | CAS#        | Qual |
| 1         | Pentadecane, 8-heptyl- | 310    | C22H46           | 071005-15-7 | 91   |
| 2         | Heneicosane            | 296    | C21H44           | 000629-94-7 | 91   |
| 3         | Tetracosane            | 338    | C24H50           | 000646-31-1 | 90   |
| 4         | Eicosane               | 282    | C20H42           | 000112-95-8 | 90   |
| 5         | Hexadecane             | 226    | C16H34           | 000544-76-3 | 86   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF122916\  
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Operator : UM/SJ  
Sample : H6301-02  
Misc :  
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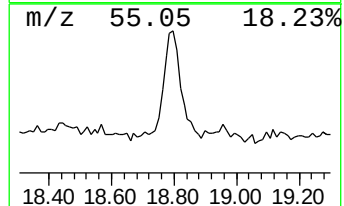
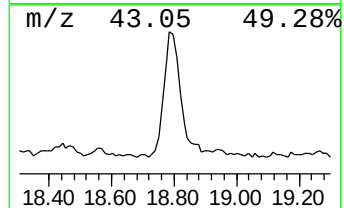
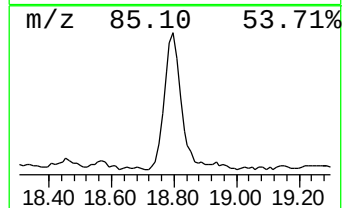
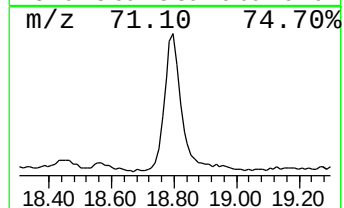
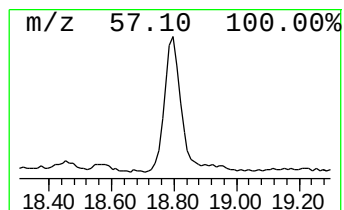
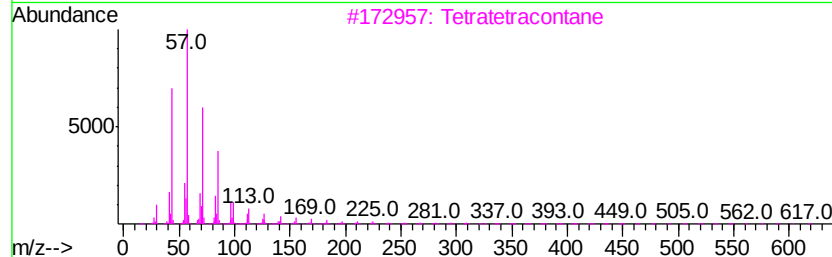
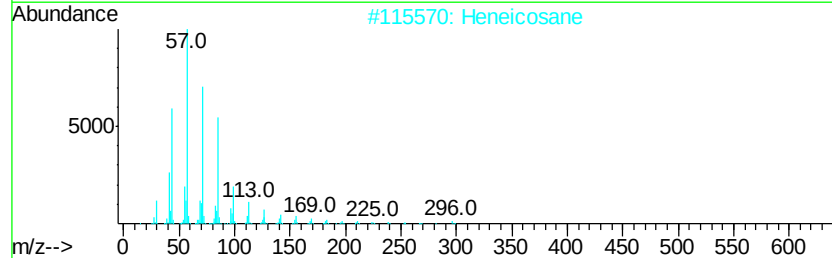
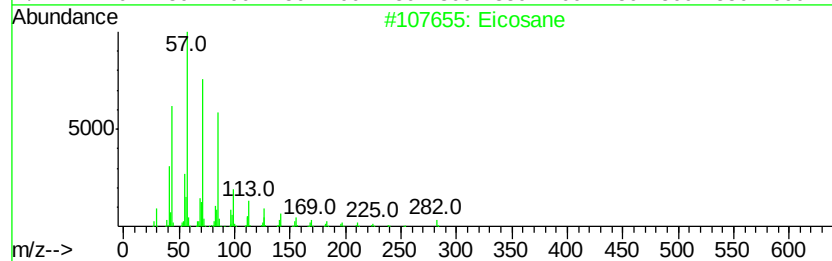
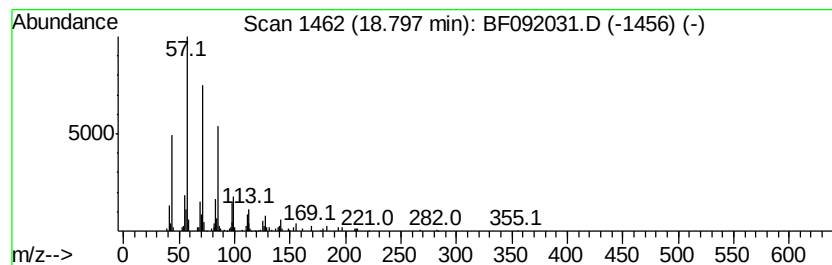
Instrument :  
BNA\_F  
ClientSampleId :  
MW-12

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 11 Eicosane Concentration Rank 10

| R.T.      | EstConc           | Area   | Relative to ISTD | R.T.        |      |
|-----------|-------------------|--------|------------------|-------------|------|
| 18.80     | 5.25 ng           | 445059 | Perylene-d12     | 15.22       |      |
| Hit# of 5 | Tentative ID      | MW     | MolForm          | CAS#        | Qual |
| 1         | Eicosane          | 282    | C20H42           | 000112-95-8 | 97   |
| 2         | Heneicosane       | 296    | C21H44           | 000629-94-7 | 91   |
| 3         | Tetratetracontane | 619    | C44H90           | 007098-22-8 | 91   |
| 4         | Heptadecane       | 240    | C17H36           | 000629-78-7 | 91   |
| 5         | Tetracosane       | 338    | C24H50           | 000646-31-1 | 91   |





Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF122916\  
Data File : BF092031.D  
Acq On : 29 Dec 2016 18:34  
Operator : UM/SJ  
Sample : H6301-02  
Misc :  
ALS Vial : 17 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
MW-12

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF122116.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.83  | 12.1    | ng    | 769432   | 1                     | 6.69  | 1269350 | 20.0 |
| unknown6.46          | 6.46  | 78.6    | ng    | 4987270  | 1                     | 6.69  | 1269350 | 20.0 |
| Heneicosane          | 14.63 | 2.7     | ng    | 225410   | 6                     | 15.22 | 1696140 | 20.0 |
| Tetracosane          | 14.92 | 5.3     | ng    | 448931   | 6                     | 15.22 | 1696140 | 20.0 |
| Pentadecane, 8-he... | 15.64 | 11.5    | ng    | 978019   | 6                     | 15.22 | 1696140 | 20.0 |
| Eicosane             | 18.80 | 5.3     | ng    | 445059   | 6                     | 15.22 | 1696140 | 20.0 |