

Data Path : Z:\HPCHEM1\BNA F\DATA\BF041318\  
 Data File : BF104482.D  
 Acq On : 13 Apr 2018 16:54  
 Operator : JU/SJ  
 Sample : J2360-01  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 NAA-WS-001

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-BF040618.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         | 5.034       | 496           | 501         | 508          | rVB      | 105396         | 143163        | 4.19%           | 0.512%        |
| 2         | 5.428       | 562           | 568         | 571          | rBV      | 2874182        | 2937853       | 85.93%          | 10.515%       |
| 3         | 6.075       | 674           | 678         | 692          | rVB      | 51342          | 88905         | 2.60%           | 0.318%        |
| 4         | 6.445       | 735           | 741         | 745          | rBV      | 2645659        | 2994792       | 87.60%          | 10.719%       |
| 5         | 6.581       | 759           | 764         | 767          | rBV      | 3093022        | 3049888       | 89.21%          | 10.916%       |
| 6         | 6.810       | 799           | 803         | 806          | rVB      | 1012771        | 788008        | 23.05%          | 2.820%        |
| 7         | 6.969       | 825           | 830         | 833          | rBV      | 2650062        | 2404590       | 70.33%          | 8.607%        |
| 8         | 7.375       | 893           | 899         | 902          | rBV      | 1837753        | 1915134       | 56.02%          | 6.855%        |
| 9         | 8.092       | 1017          | 1021        | 1024         | rBV      | 1311547        | 1050980       | 30.74%          | 3.762%        |
| 10        | 9.169       | 1199          | 1204        | 1208         | rBV      | 3341086        | 3418866       | 100.00%         | 12.237%       |
| 11        | 9.563       | 1267          | 1271        | 1274         | rBV      | 485403         | 391793        | 11.46%          | 1.402%        |
| 12        | 9.775       | 1304          | 1307        | 1311         | rVB      | 124269         | 94150         | 2.75%           | 0.337%        |
| 13        | 9.851       | 1316          | 1320        | 1328         | rVB      | 1332849        | 1140264       | 33.35%          | 4.081%        |
| 14        | 10.275      | 1389          | 1392        | 1395         | rVB      | 130267         | 107789        | 3.15%           | 0.386%        |
| 15        | 10.498      | 1424          | 1430        | 1432         | rBV      | 32182          | 41584         | 1.22%           | 0.149%        |
| 16        | 10.639      | 1450          | 1454        | 1458         | rBV      | 1883782        | 1839432       | 53.80%          | 6.584%        |
| 17        | 10.751      | 1470          | 1473        | 1478         | rBV      | 113063         | 113819        | 3.33%           | 0.407%        |
| 18        | 11.198      | 1546          | 1549        | 1553         | rBV      | 52940          | 49227         | 1.44%           | 0.176%        |
| 19        | 11.339      | 1569          | 1573        | 1576         | rBV      | 1241930        | 1017230       | 29.75%          | 3.641%        |
| 20        | 12.927      | 1838          | 1843        | 1847         | rBV      | 2545983        | 2659887       | 77.80%          | 9.520%        |
| 21        | 13.816      | 1991          | 1994        | 1998         | rBV      | 310789         | 303711        | 8.88%           | 1.087%        |
| 22        | 13.986      | 2019          | 2023        | 2026         | rBV      | 794939         | 724477        | 21.19%          | 2.593%        |
| 23        | 15.451      | 2268          | 2272        | 2281         | rBV      | 494379         | 663060        | 19.39%          | 2.373%        |

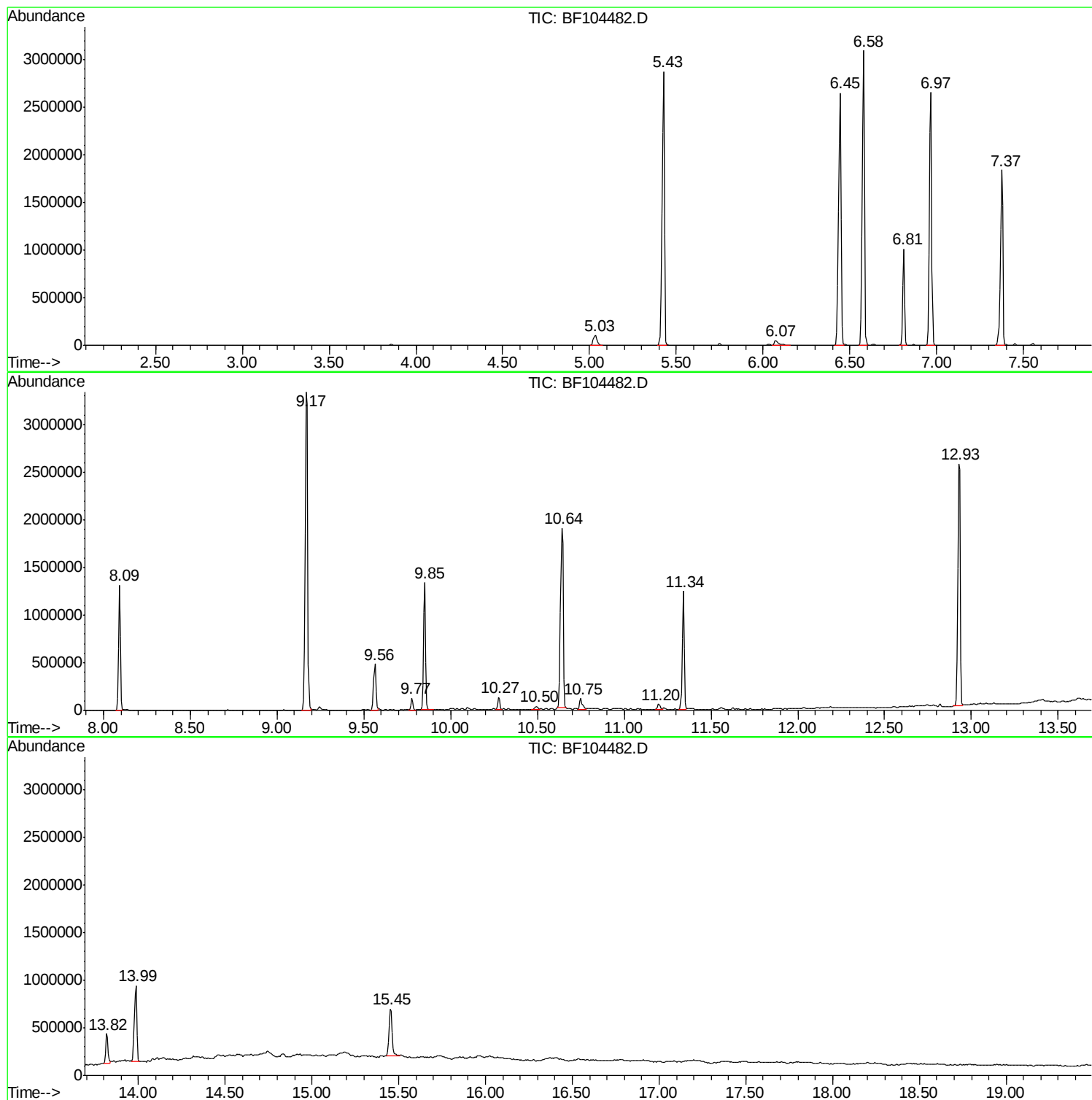
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Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
NAA-WS-001

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF040618.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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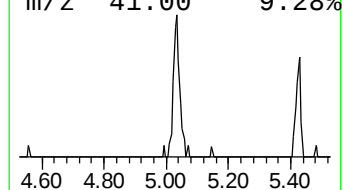
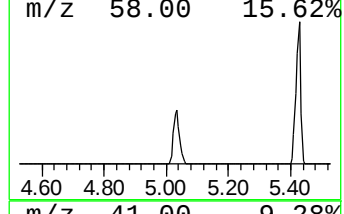
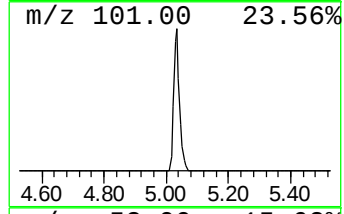
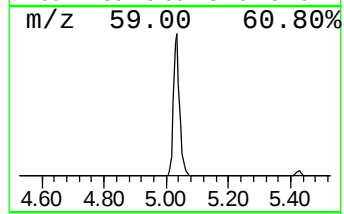
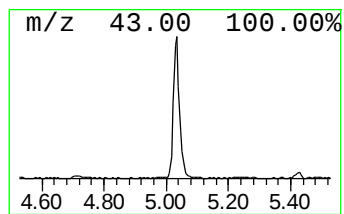
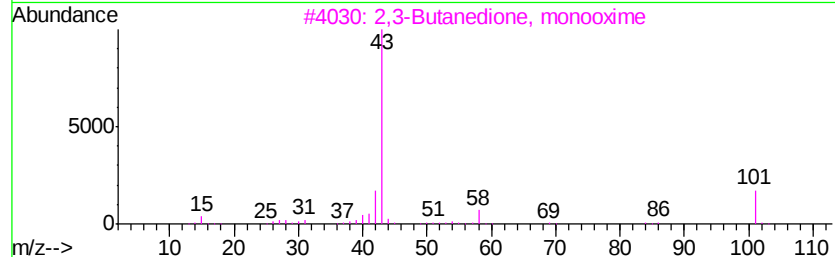
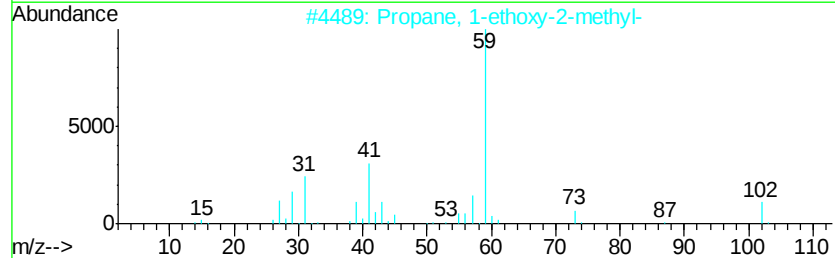
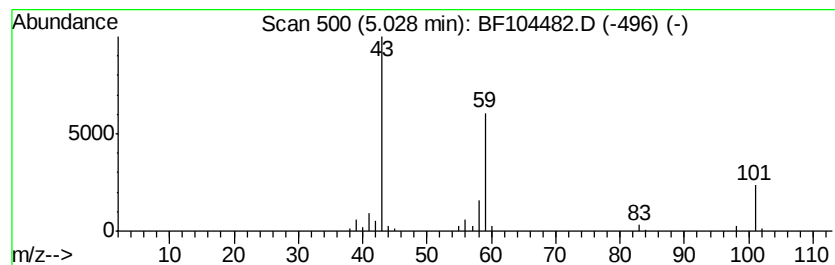
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TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.03 | 3.63 ng | 143163 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# | of | 5 | Tentative ID                         | MW  | MolForm  | CAS#        | Qual |
|------|----|---|--------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-     | 116 | C6H12O2  | 000123-42-2 | 72   |
| 2    |    |   | Propane, 1-ethoxy-2-methyl-          | 102 | C6H14O   | 000627-02-1 | 43   |
| 3    |    |   | 2,3-Butanedione, monooxime           | 101 | C4H7NO2  | 000057-71-6 | 25   |
| 4    |    |   | Acetic acid, cyano-, 1,1-dimethyl... | 141 | C7H11NO2 | 001116-98-9 | 17   |
| 5    |    |   | Morpholine, 4-methyl-                | 101 | C5H11NO  | 000109-02-4 | 9    |



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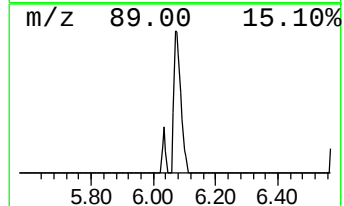
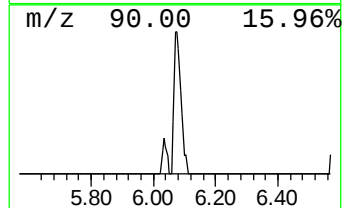
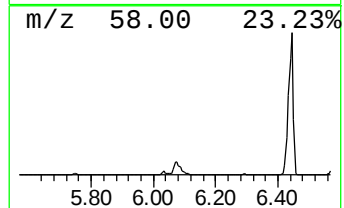
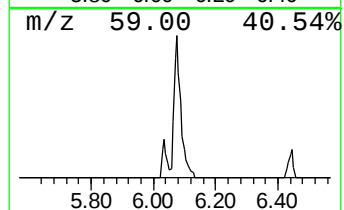
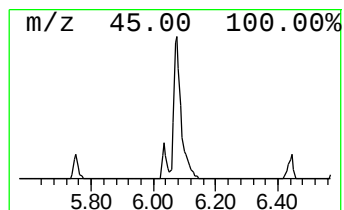
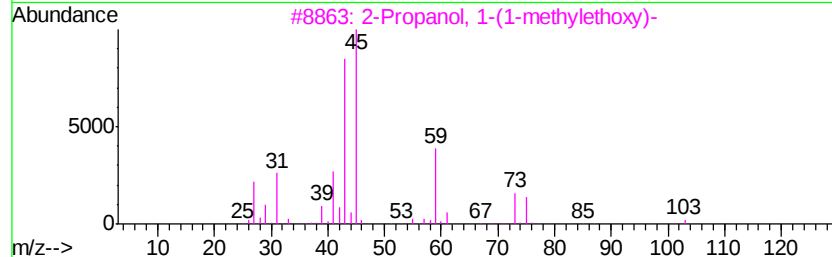
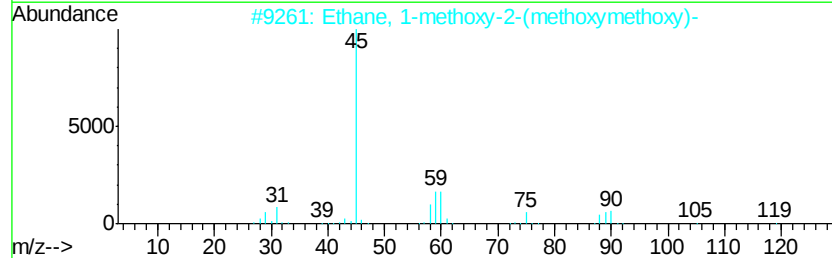
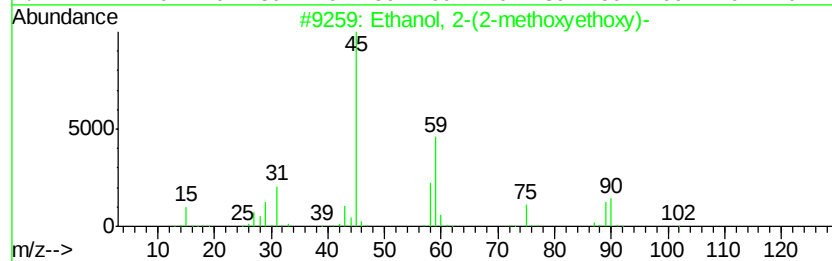
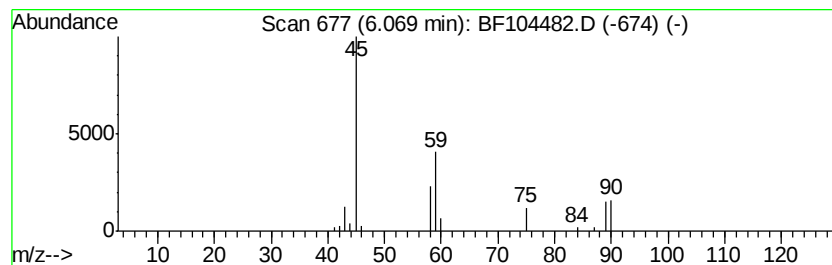
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 5

| R.T. | EstConc | Area  | Relative to ISTD       | R.T. |
|------|---------|-------|------------------------|------|
| 6.07 | 2.26 ng | 88905 | 1,4-Dichlorobenzene-d4 | 6.81 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|---------|---|-------------------------------------|-----|---------|-------------|------|
| 1       |   | Ethanol, 2-(2-methoxyethoxy)-       | 120 | C5H12O3 | 000111-77-3 | 74   |
| 2       |   | Ethane, 1-methoxy-2-(methoxymeth... | 120 | C5H12O3 | 074498-88-7 | 40   |
| 3       |   | 2-Propanol, 1-(1-methylethoxy)-     | 118 | C6H14O2 | 003944-36-3 | 38   |
| 4       |   | Paraldehyde                         | 132 | C6H12O3 | 000123-63-7 | 9    |
| 5       |   | Carbonic acid, dimethyl ester       | 90  | C3H6O3  | 000616-38-6 | 9    |



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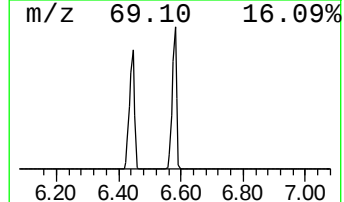
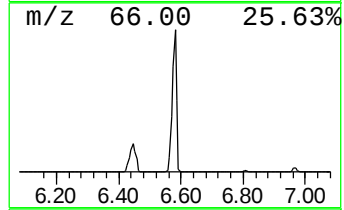
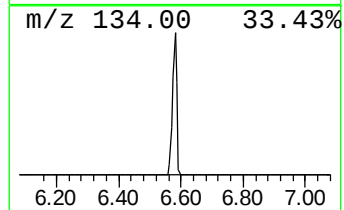
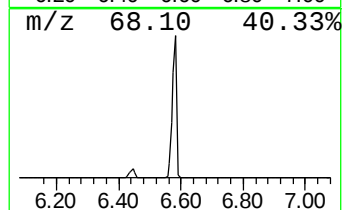
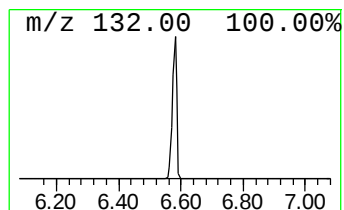
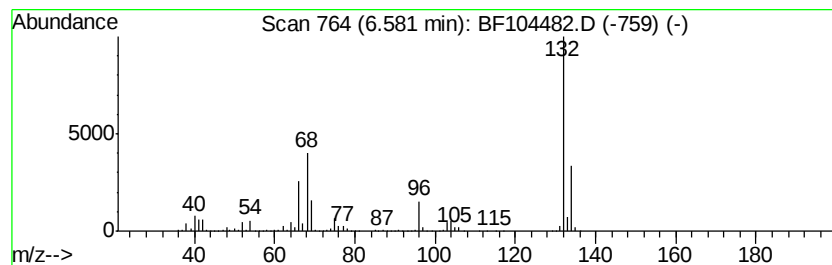
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 3 unknown6.58 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.58 | 77.41 ng | 3049890 | 1,4-Dichlorobenzene-d4 | 6.81 |

| 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    |    | Tranvlcypropine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | 4-Chloro-2-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-00-5  | 9    |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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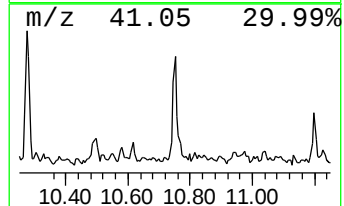
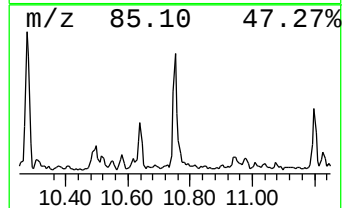
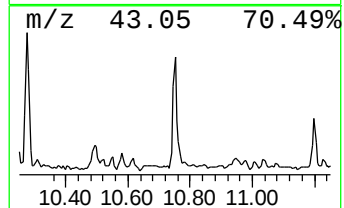
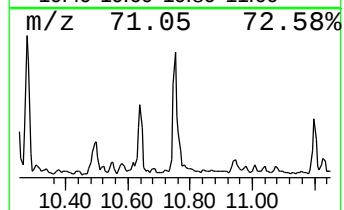
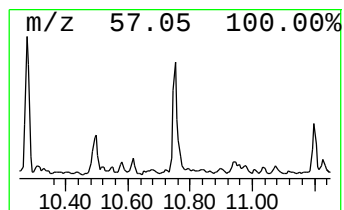
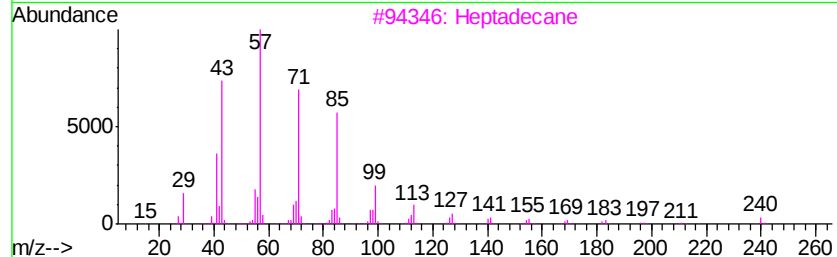
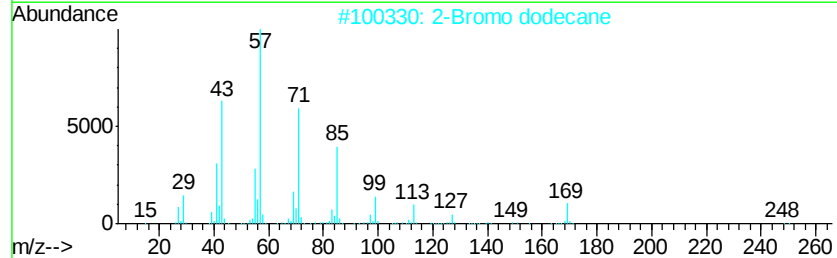
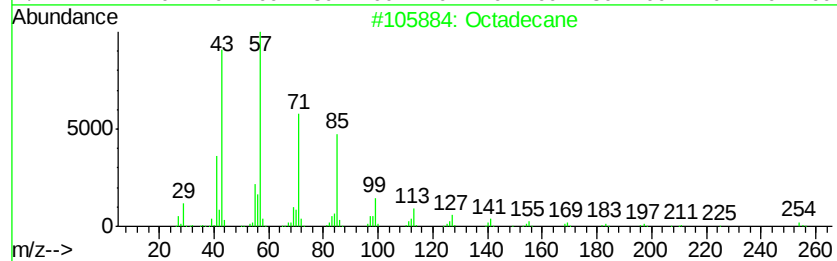
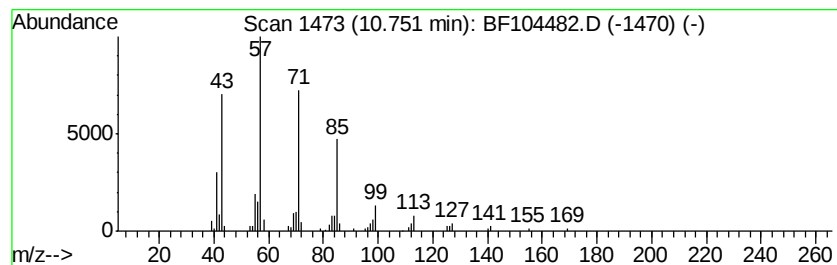
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Octadecane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 10.75 | 2.24 ng | 113819 | Phenanthrene-d10 | 11.34 |

| Hit# of | 5                | Tentative ID | MW  | MolForm  | CAS#        | Qual |
|---------|------------------|--------------|-----|----------|-------------|------|
| 1       | Octadecane       |              | 254 | C18H38   | 000593-45-3 | 91   |
| 2       | 2-Bromo dodecane |              | 248 | C12H25Br | 013187-99-0 | 90   |
| 3       | Heptadecane      |              | 240 | C17H36   | 000629-78-7 | 90   |
| 4       | Tetradecane      |              | 198 | C14H30   | 000629-59-4 | 87   |
| 5       | Eicosane         |              | 282 | C20H42   | 000112-95-8 | 86   |



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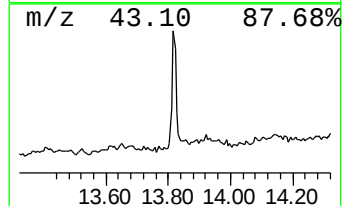
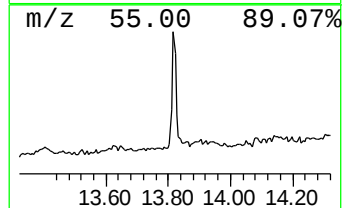
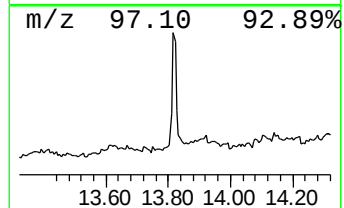
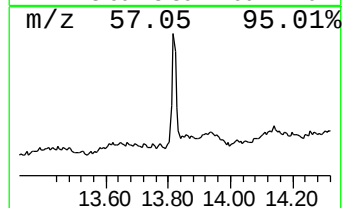
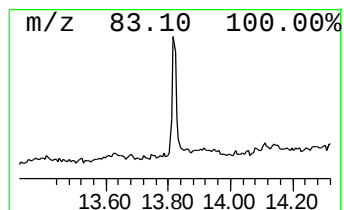
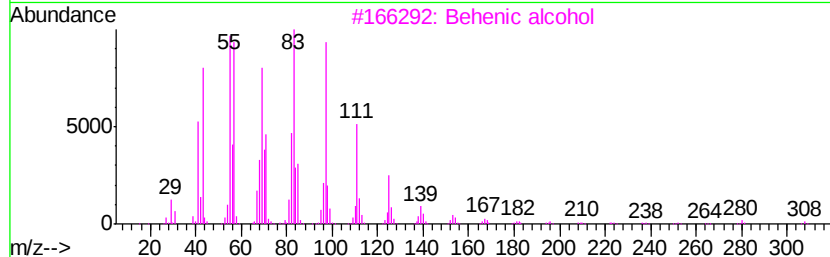
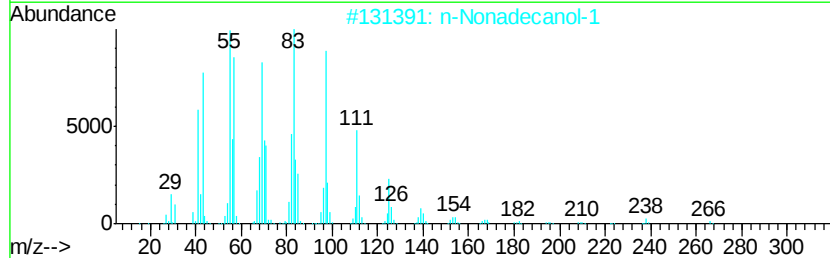
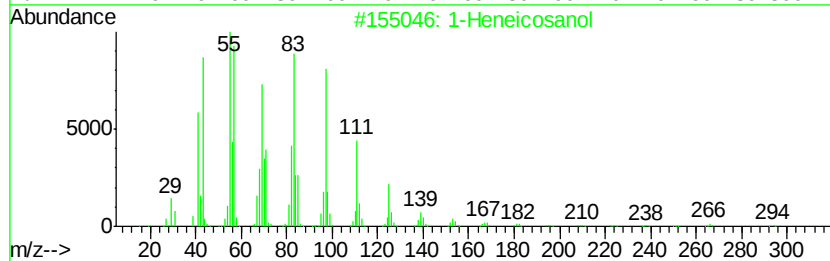
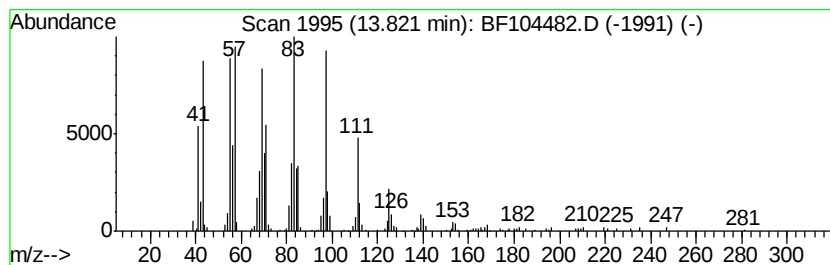
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 1-Heneicosanol Concentration Rank 3

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.82 | 8.38 ng | 303711 | Chrysene-d12     | 13.99 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 1-Heneicosanol                      | 312 | C21H44O    | 015594-90-8 | 95   |
| 2    |    | n-Nonadecanol-1                     | 284 | C19H40O    | 001454-84-8 | 95   |
| 3    |    | Behenic alcohol                     | 326 | C22H46O    | 000661-19-8 | 94   |
| 4    |    | Pentafluoropropionic acid, penta... | 374 | C18H31F5O2 | 959092-08-1 | 93   |
| 5    |    | Trifluoroacetic acid, pentadecyl... | 324 | C17H31F3O2 | 959010-23-2 | 93   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.03  | 3.6     | ng    | 143163   | 1                     | 6.81  | 788008  | 20.0 |
| Ethanol, 2-(2-met... | 6.07  | 2.3     | ng    | 88905    | 1                     | 6.81  | 788008  | 20.0 |
| unknown6.58          | 6.58  | 77.4    | ng    | 3049890  | 1                     | 6.81  | 788008  | 20.0 |
| Octadecane           | 10.75 | 2.2     | ng    | 113819   | 4                     | 11.34 | 1017230 | 20.0 |
| 1-Heneicosanol       | 13.82 | 8.4     | ng    | 303711   | 5                     | 13.99 | 724477  | 20.0 |