

Data Path : Z:\HPCHEM1\BNA F\DATA\BF081217\  
 Data File : BF097635.D  
 Acq On : 12 Aug 2017 15:24  
 Operator : SJ/JU  
 Sample : PB101441BL  
 Misc :  
 ALS Vial : 4 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 PB101441BL

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-BF081117.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         | 4.792       | 523           | 528         | 550          | rBV2     | 116017         | 369277        | 9.78%           | 1.203%        |
| 2         | 5.434       | 632           | 637         | 669          | rBV      | 2150101        | 3733867       | 98.86%          | 12.164%       |
| 3         | 7.063       | 908           | 914         | 925          | rBV      | 2086803        | 3447360       | 91.27%          | 11.230%       |
| 4         | 7.157       | 925           | 930         | 940          | rVB      | 2174910        | 3446130       | 91.24%          | 11.226%       |
| 5         | 7.498       | 984           | 988         | 1006         | rVB      | 501010         | 713240        | 18.88%          | 2.323%        |
| 6         | 7.733       | 1023          | 1028        | 1048         | rBV      | 1738577        | 2534992       | 67.12%          | 8.258%        |
| 7         | 8.410       | 1137          | 1143        | 1169         | rBV      | 1325225        | 2251163       | 59.60%          | 7.334%        |
| 8         | 9.527       | 1328          | 1333        | 1362         | rBV      | 675931         | 1075529       | 28.48%          | 3.504%        |
| 9         | 11.304      | 1627          | 1635        | 1653         | rBV      | 2268875        | 3777017       | 100.00%         | 12.304%       |
| 10        | 12.345      | 1806          | 1812        | 1825         | rBV2     | 716506         | 1090675       | 28.88%          | 3.553%        |
| 11        | 13.645      | 2027          | 2033        | 2052         | rBV      | 1233596        | 1906301       | 50.47%          | 6.210%        |
| 12        | 14.745      | 2215          | 2220        | 2236         | rBV2     | 656476         | 962426        | 25.48%          | 3.135%        |
| 13        | 17.109      | 2615          | 2622        | 2625         | rBV2     | 2174034        | 3024692       | 80.08%          | 9.853%        |
| 14        | 18.444      | 2844          | 2849        | 2859         | rBV      | 849202         | 1015089       | 26.88%          | 3.307%        |
| 15        | 19.874      | 3088          | 3092        | 3096         | rBV      | 43466          | 48388         | 1.28%           | 0.158%        |
| 16        | 20.109      | 3128          | 3132        | 3142         | rBV      | 602894         | 768678        | 20.35%          | 2.504%        |
| 17        | 20.209      | 3145          | 3149        | 3155         | rVV      | 75320          | 96866         | 2.56%           | 0.316%        |
| 18        | 20.562      | 3205          | 3209        | 3214         | rVB      | 92565          | 110241        | 2.92%           | 0.359%        |
| 19        | 20.956      | 3271          | 3276        | 3281         | rVB2     | 70693          | 117838        | 3.12%           | 0.384%        |
| 20        | 21.403      | 3347          | 3352        | 3358         | rBV      | 57764          | 98804         | 2.62%           | 0.322%        |
| 21        | 21.927      | 3436          | 3441        | 3448         | rBV2     | 35251          | 66035         | 1.75%           | 0.215%        |
| 22        | 22.544      | 3542          | 3546        | 3557         | rVB8     | 17888          | 42225         | 1.12%           | 0.138%        |

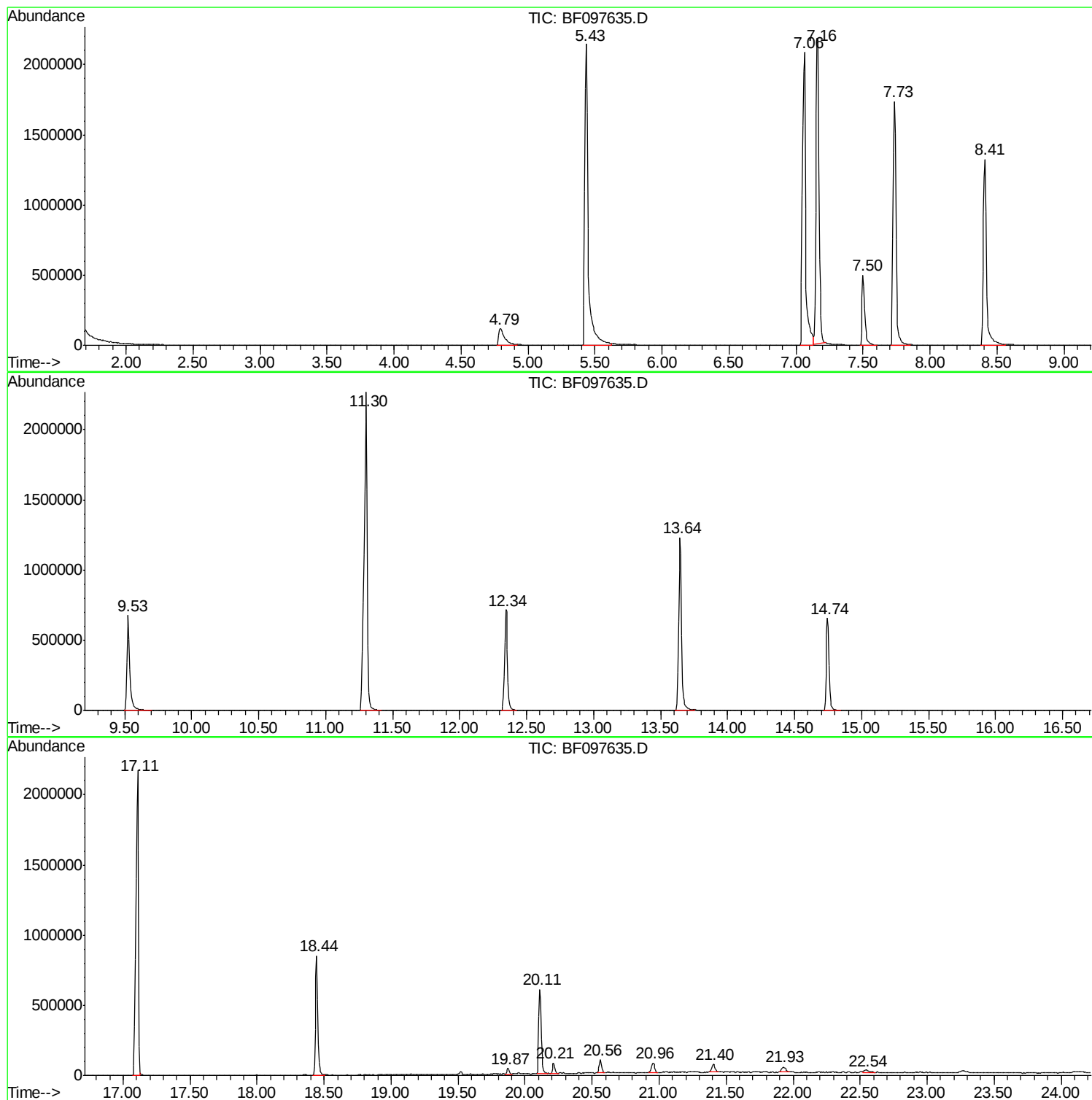
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Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB101441BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081117.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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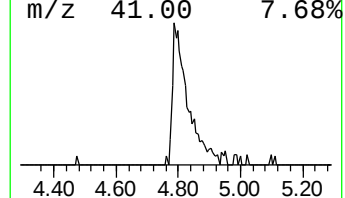
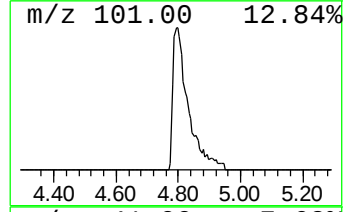
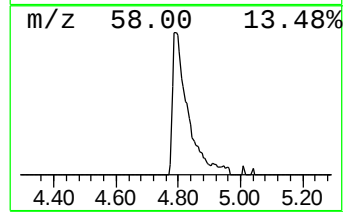
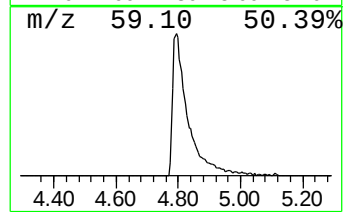
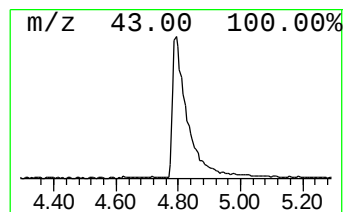
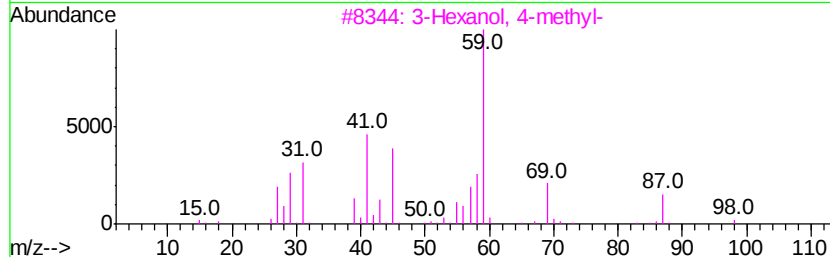
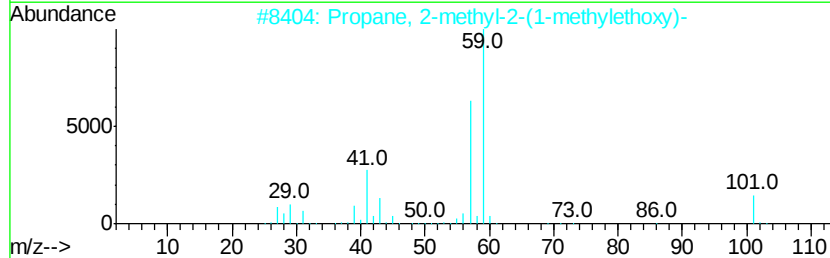
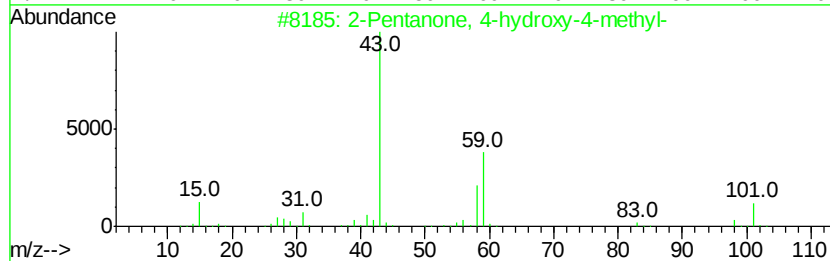
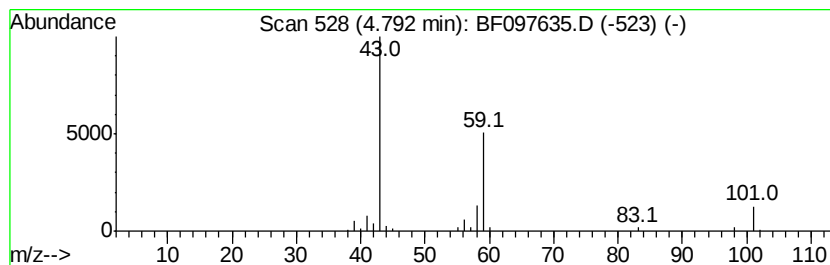
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.79 | 10.35 ng | 369277 | 1,4-Dichlorobenzene-d4 | 7.50 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 64   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 36   |
| 3    |    |   | 3-Hexanol, 4-methyl-                | 116 | C7H16O   | 000615-29-2 | 33   |
| 4    |    |   | 2-Hexanol, 2-methyl-                | 116 | C7H16O   | 000625-23-0 | 33   |
| 5    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 25   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

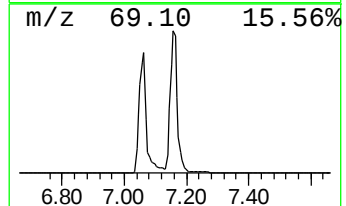
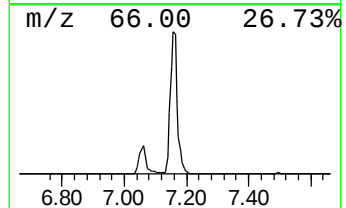
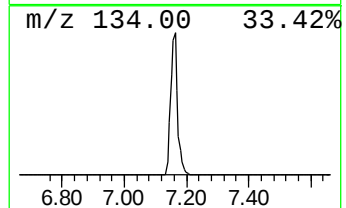
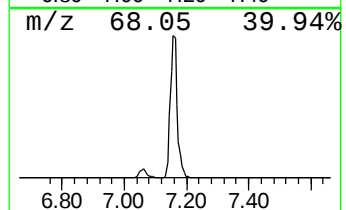
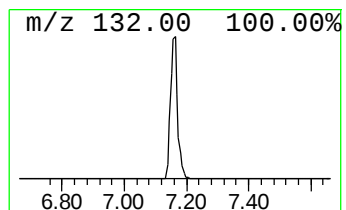
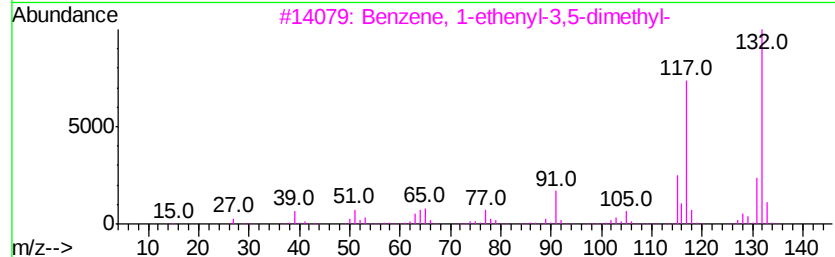
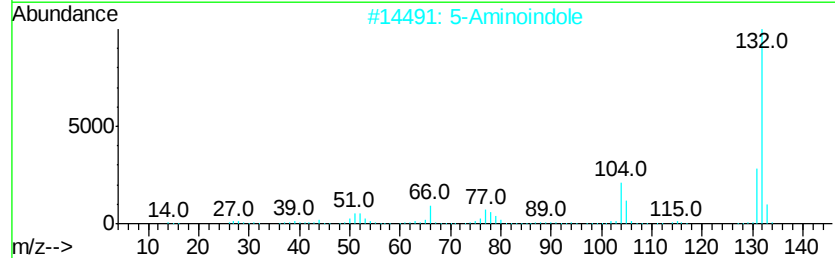
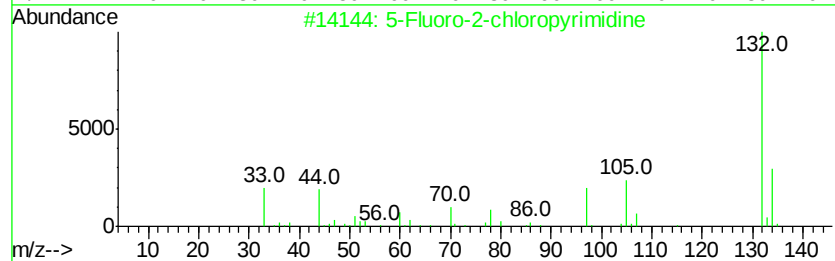
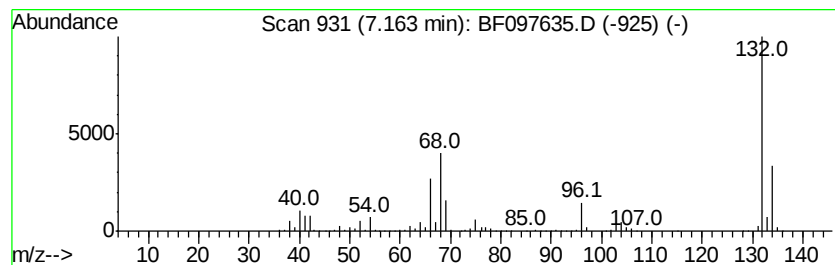
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.16 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.16 | 96.63 ng | 3446130 | 1,4-Dichlorobenzene-d4 | 7.50 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0 | 16   |
| 2    |    | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0 | 12   |
| 3    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4 | 9    |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6 | 9    |
| 5    |    | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9 | 9    |



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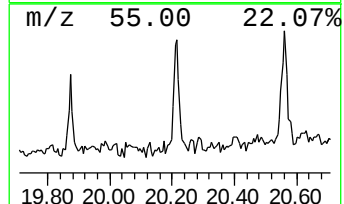
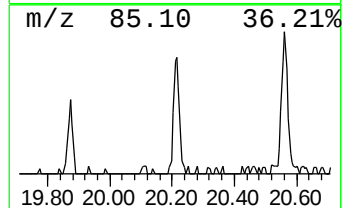
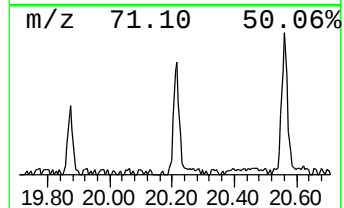
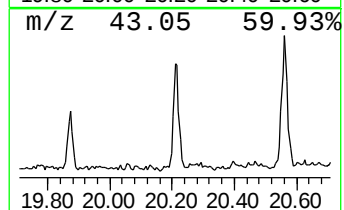
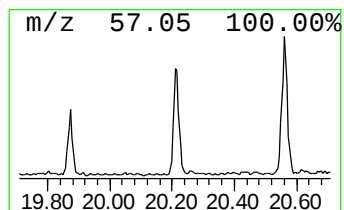
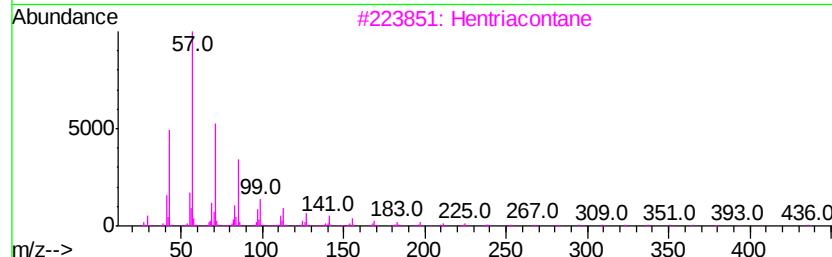
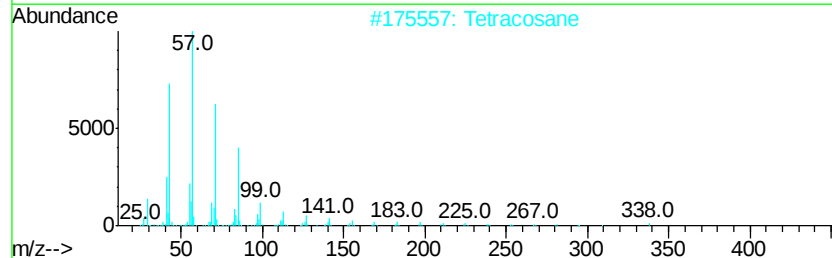
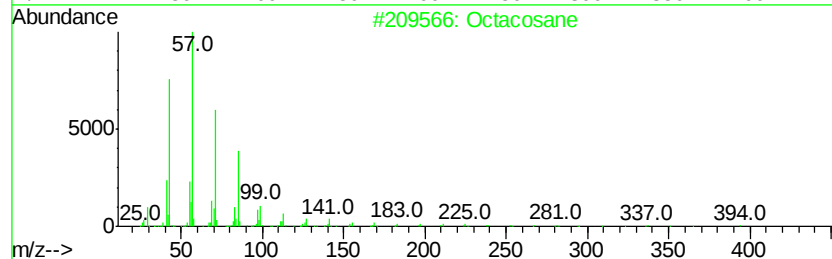
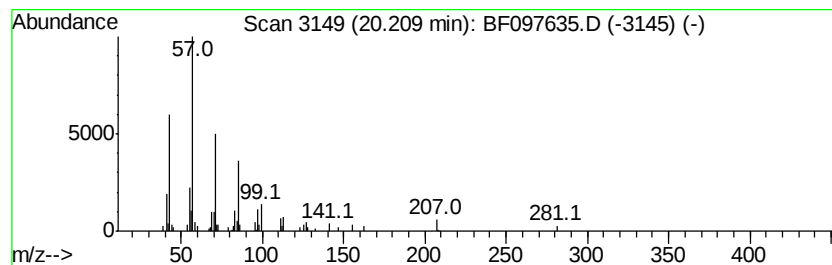
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Octacosane Concentration Rank 7

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 20.21 | 2.52 ng | 96866 | Perylene-d12     | 20.11 |

| Hit# | of | Tentative ID   | MW  | MolForm | CAS#        | Qual |
|------|----|----------------|-----|---------|-------------|------|
| 1    | 5  | Octacosane     | 394 | C28H58  | 000630-02-4 | 90   |
| 2    |    | Tetracosane    | 338 | C24H50  | 000646-31-1 | 87   |
| 3    |    | Hentriacontane | 437 | C31H64  | 000630-04-6 | 86   |
| 4    |    | Hexacosane     | 366 | C26H54  | 000630-01-3 | 83   |
| 5    |    | Heptacosane    | 380 | C27H56  | 000593-49-7 | 83   |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

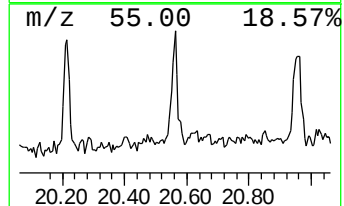
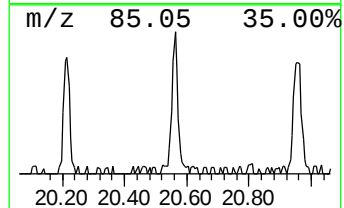
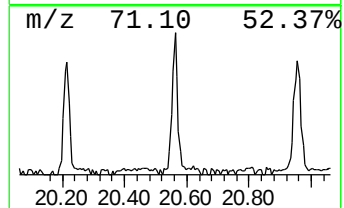
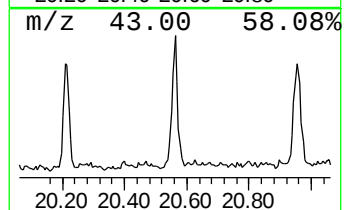
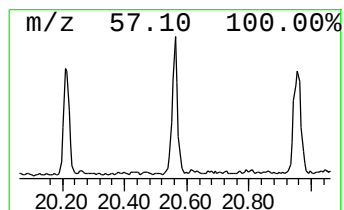
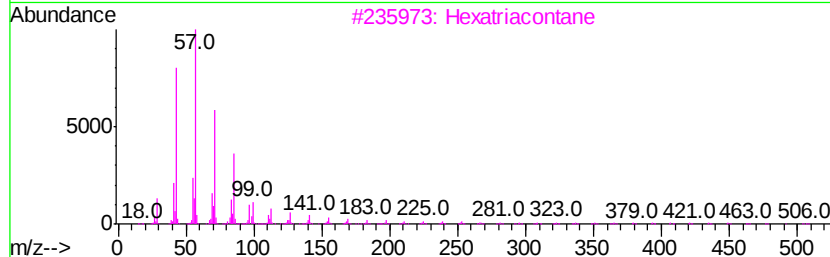
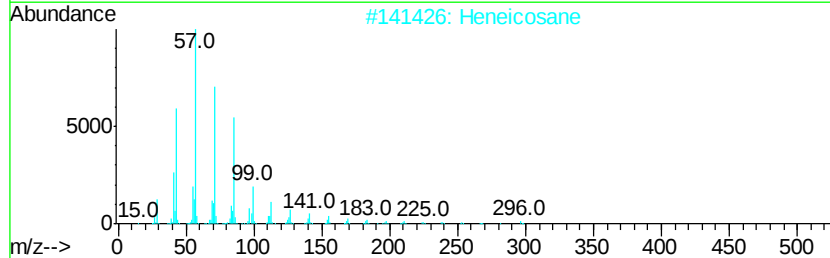
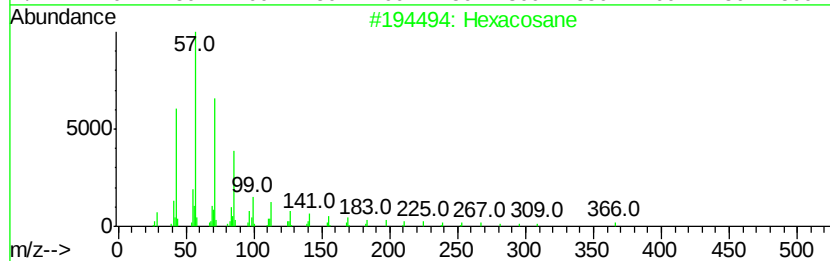
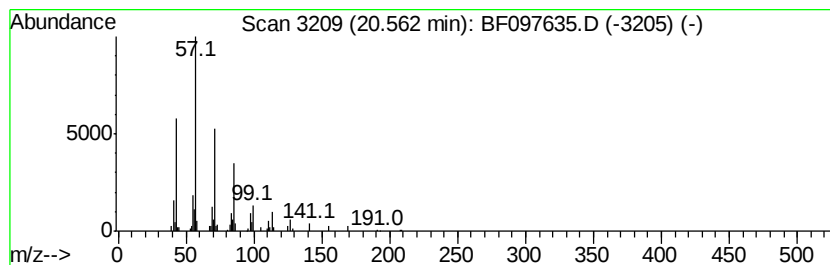
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 Hexacosane Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.56 | 2.87 ng | 110241 | Perylene-d12     | 20.11 |

| Hit# of | 5                  | Tentative ID | MW  | MolForm | CAS#         | Qual |
|---------|--------------------|--------------|-----|---------|--------------|------|
| 1       | Hexacosane         |              | 366 | C26H54  | 000630-01-3  | 90   |
| 2       | Heneicosane        |              | 296 | C21H44  | 000629-94-7  | 87   |
| 3       | Hexatriacontane    |              | 507 | C36H74  | 000630-06-8  | 86   |
| 4       | Tetratetracontane  |              | 619 | C44H90  | 007098-22-8  | 86   |
| 5       | 2-methyloctacosane |              | 408 | C29H60  | 1000376-72-8 | 83   |



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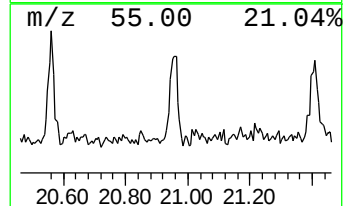
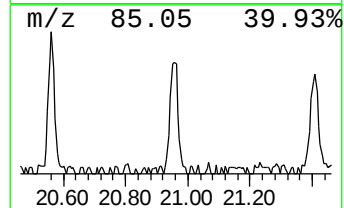
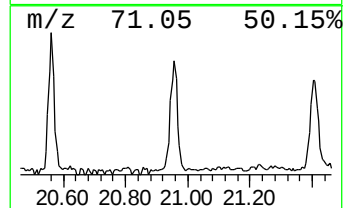
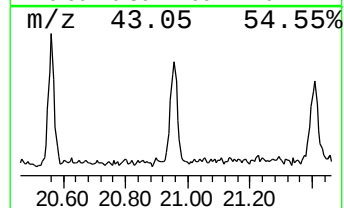
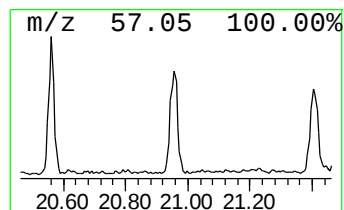
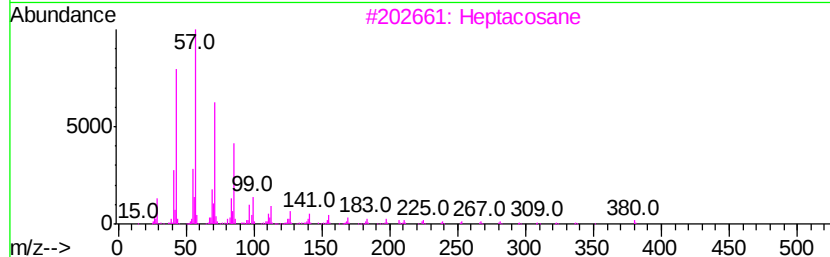
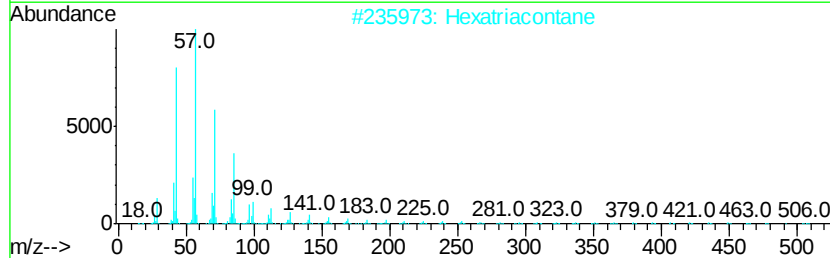
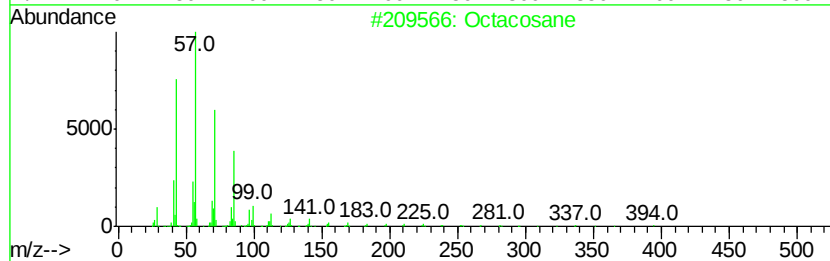
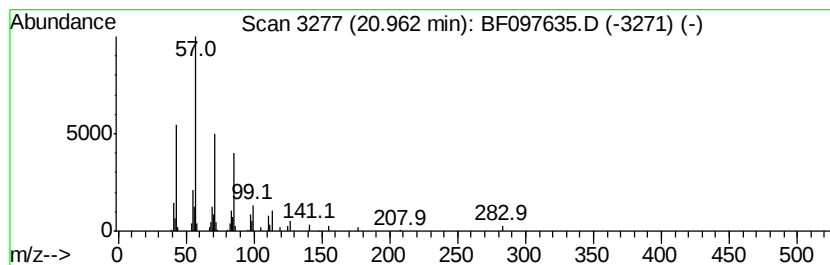
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Hexatriacontane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 20.96 | 3.07 ng | 117838 | Perylene-d12     | 20.11 |

| Hit# | of | Tentative ID    | MW  | MolForm | CAS#        | Qual |
|------|----|-----------------|-----|---------|-------------|------|
| 1    | 5  | Octacosane      | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    | Hexatriacontane | 507 | C36H74  | 000630-06-8 | 91   |
| 3    |    | Heptacosane     | 380 | C27H56  | 000593-49-7 | 90   |
| 4    |    | Hentriacontane  | 437 | C31H64  | 000630-04-6 | 90   |
| 5    |    | Hexacosane      | 366 | C26H54  | 000630-01-3 | 87   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF081217\  
Data File : BF097635.D  
Acq On : 12 Aug 2017 15:24  
Operator : SJ/JU  
Sample : PB101441BL  
Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB101441BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

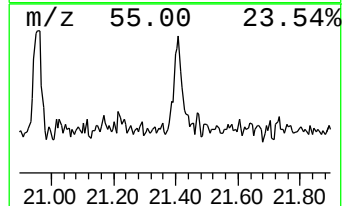
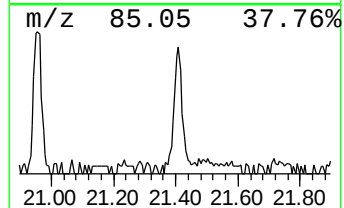
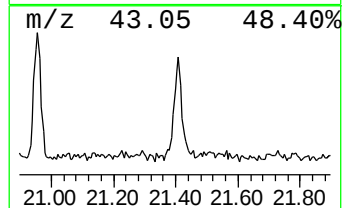
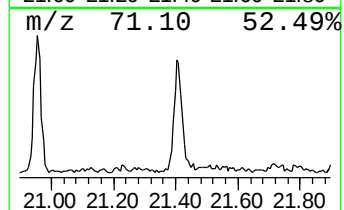
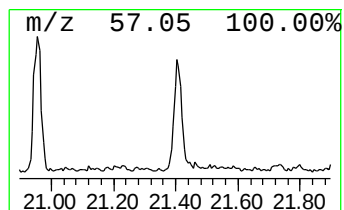
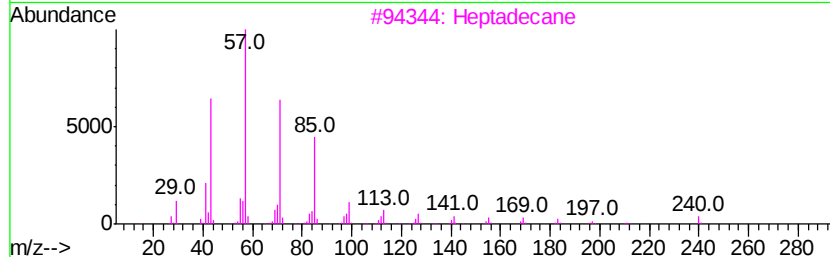
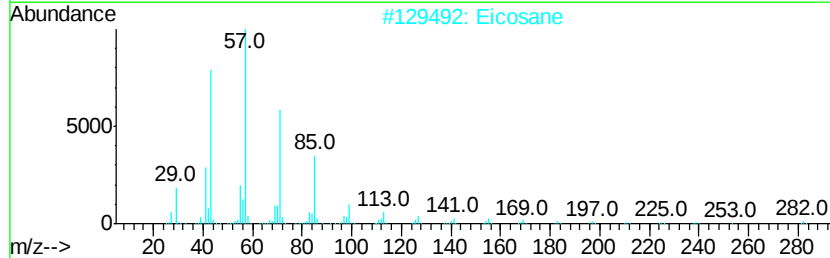
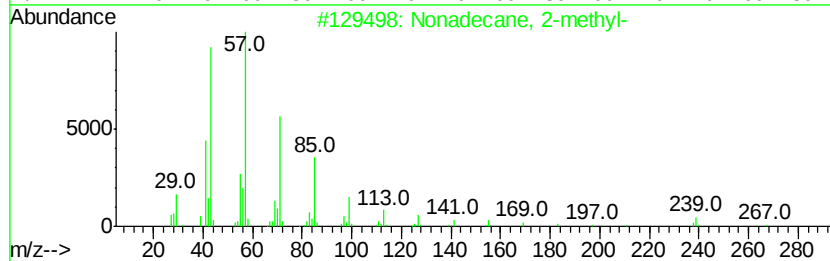
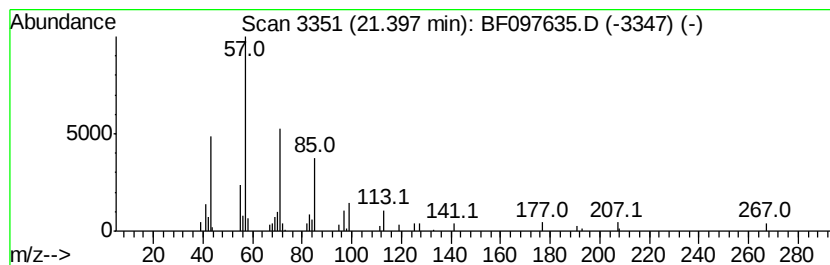
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 7 Nonadecane, 2-methyl- Concentration Rank 6

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 21.40 | 2.57 ng | 98804 | Perylene-d12     | 20.11 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | Nonadecane, 2-methyl-               | 282 | C20H42  | 001560-86-7 | 86   |
| 2    |    | Eicosane                            | 282 | C20H42  | 000112-95-8 | 86   |
| 3    |    | Heptadecane                         | 240 | C17H36  | 000629-78-7 | 80   |
| 4    |    | Heneicosane                         | 296 | C21H44  | 000629-94-7 | 74   |
| 5    |    | Heptadecane, 2,6,10,15-tetramethyl- | 296 | C21H44  | 054833-48-6 | 72   |



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Misc :  
ALS Vial : 4 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
PB101441BL

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF081117.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| 2-Pentanone, 4-hy... | 4.79  | 10.4    | ng    | 369277   | 1                     | 7.50  | 713240 | 20.0 |
| unknown7.16          | 7.16  | 96.6    | ng    | 3446130  | 1                     | 7.50  | 713240 | 20.0 |
| Octacosane           | 20.21 | 2.5     | ng    | 96866    | 6                     | 20.11 | 768678 | 20.0 |
| Hexacosane           | 20.56 | 2.9     | ng    | 110241   | 6                     | 20.11 | 768678 | 20.0 |
| Hexatriacontane      | 20.96 | 3.1     | ng    | 117838   | 6                     | 20.11 | 768678 | 20.0 |
| Nonadecane, 2-met... | 21.40 | 2.6     | ng    | 98804    | 6                     | 20.11 | 768678 | 20.0 |