

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF050617\  
 Data File : BF094971.D  
 Acq On : 8 May 2017 6:14  
 Operator : SJ/MA  
 Sample : I2947-18  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-06-4.5-5.0

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-BF050217.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         | 5.043       | 524           | 528         | 549          | rBV      | 158869         | 324451        | 9.90%           | 1.252%        |
| 2         | 5.666       | 630           | 634         | 666          | rBV      | 1749144        | 2736650       | 83.51%          | 10.563%       |
| 3         | 7.266       | 900           | 906         | 921          | rBV      | 1981581        | 2899264       | 88.47%          | 11.191%       |
| 4         | 7.384       | 921           | 926         | 936          | rVB      | 2397058        | 3129302       | 95.49%          | 12.078%       |
| 5         | 7.719       | 979           | 983         | 993          | rBV      | 528937         | 604869        | 18.46%          | 2.335%        |
| 6         | 7.960       | 1019          | 1024        | 1039         | rBV      | 2007636        | 2341609       | 71.45%          | 9.038%        |
| 7         | 8.619       | 1131          | 1136        | 1156         | rBV      | 1212113        | 1708402       | 52.13%          | 6.594%        |
| 8         | 9.736       | 1322          | 1326        | 1347         | rBV      | 575571         | 802988        | 24.50%          | 3.099%        |
| 9         | 11.519      | 1623          | 1629        | 1642         | rBV      | 2447679        | 3277117       | 100.00%         | 12.649%       |
| 10        | 12.201      | 1741          | 1745        | 1753         | rBV      | 307725         | 400210        | 12.21%          | 1.545%        |
| 11        | 12.566      | 1803          | 1807        | 1819         | rBV2     | 605346         | 891457        | 27.20%          | 3.441%        |
| 12        | 13.413      | 1947          | 1951        | 1956         | rBV2     | 40999          | 44440         | 1.36%           | 0.172%        |
| 13        | 13.866      | 2022          | 2028        | 2043         | rBV      | 1183718        | 1743207       | 53.19%          | 6.728%        |
| 14        | 14.183      | 2078          | 2082        | 2085         | rBV      | 39214          | 50255         | 1.53%           | 0.194%        |
| 15        | 14.971      | 2211          | 2216        | 2233         | rBV      | 564013         | 796539        | 24.31%          | 3.074%        |
| 16        | 15.936      | 2375          | 2380        | 2388         | rBV      | 84408          | 124020        | 3.78%           | 0.479%        |
| 17        | 17.142      | 2581          | 2585        | 2589         | rVB2     | 44706          | 46033         | 1.40%           | 0.178%        |
| 18        | 17.295      | 2605          | 2611        | 2619         | rBV2     | 2042215        | 2479495       | 75.66%          | 9.570%        |
| 19        | 18.601      | 2826          | 2833        | 2834         | rBV5     | 27507          | 51278         | 1.56%           | 0.198%        |
| 20        | 18.636      | 2835          | 2839        | 2854         | rVB      | 541294         | 725665        | 22.14%          | 2.801%        |
| 21        | 20.300      | 3118          | 3122        | 3132         | rBV      | 488200         | 625201        | 19.08%          | 2.413%        |
| 22        | 20.771      | 3199          | 3202        | 3206         | rVB2     | 26178          | 34531         | 1.05%           | 0.133%        |
| 23        | 20.889      | 3216          | 3222        | 3226         | rBV8     | 18360          | 37037         | 1.13%           | 0.143%        |
| 24        | 21.200      | 3271          | 3275        | 3278         | rBV3     | 20914          | 34019         | 1.04%           | 0.131%        |

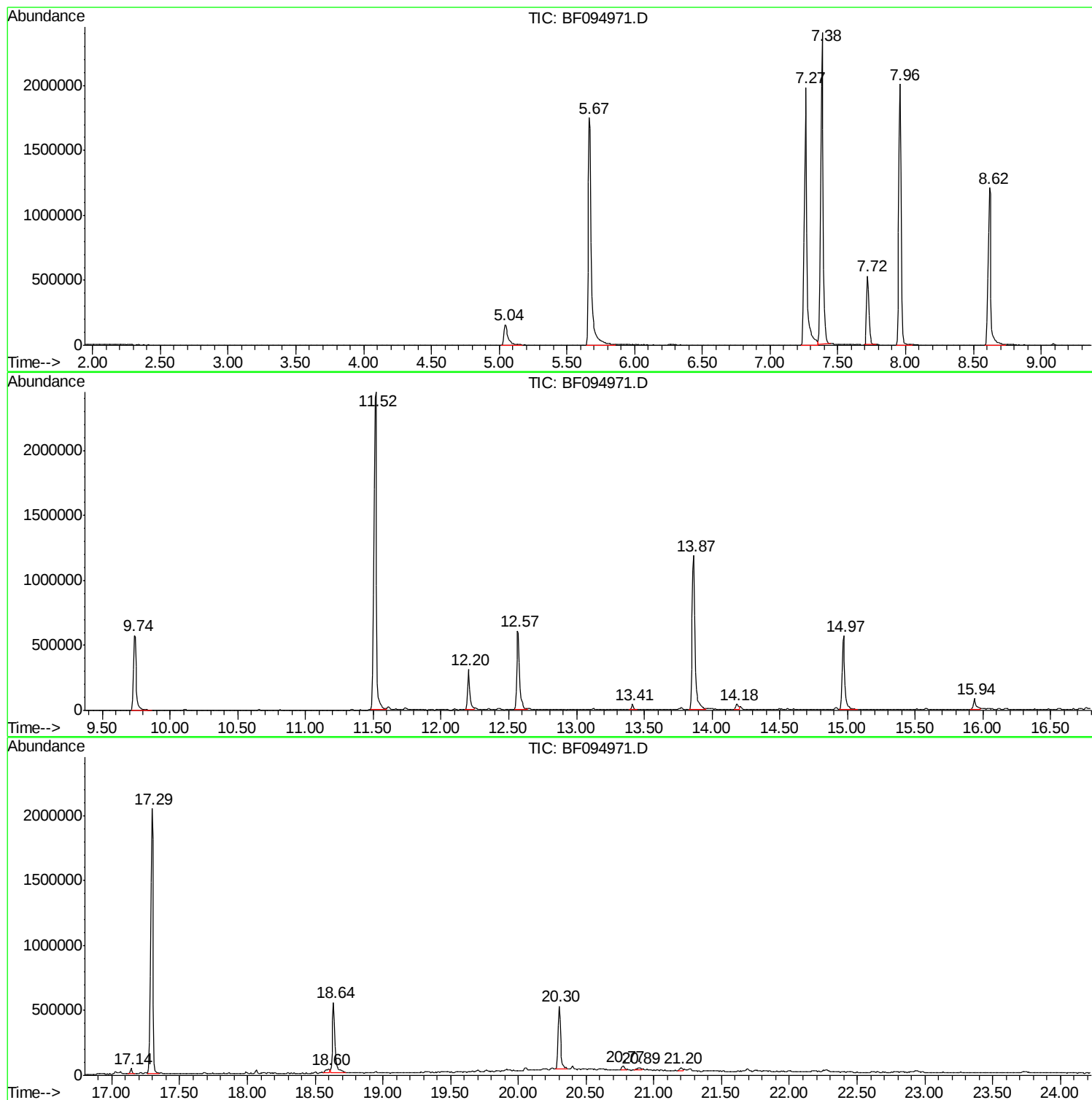
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Instrument :  
BNA\_F  
ClientSampled :  
SB-06-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.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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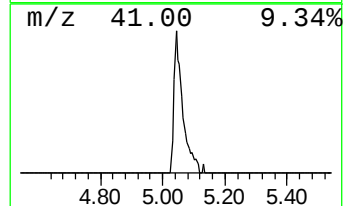
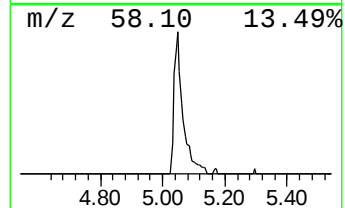
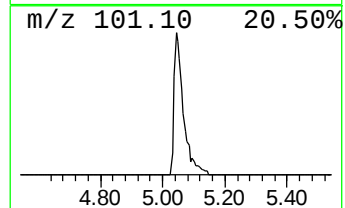
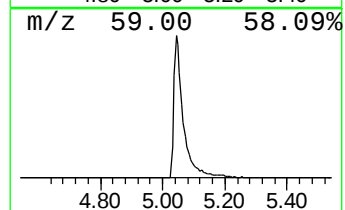
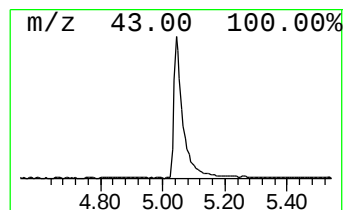
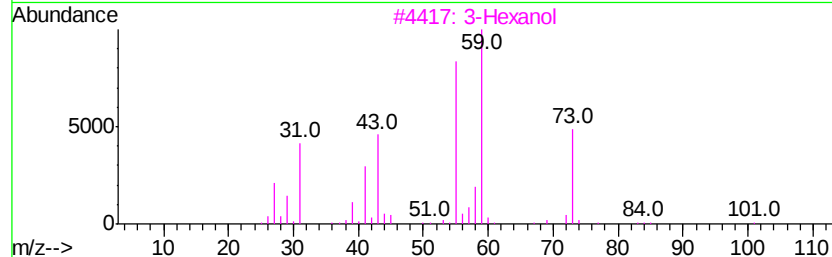
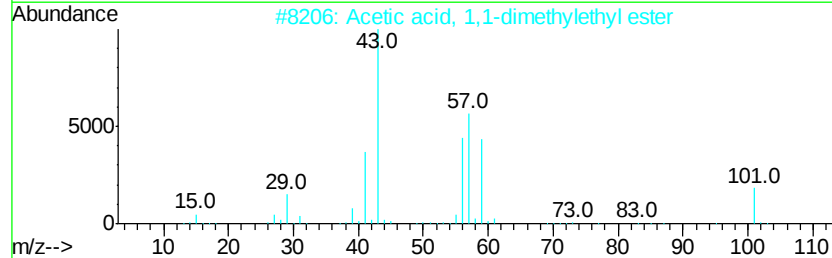
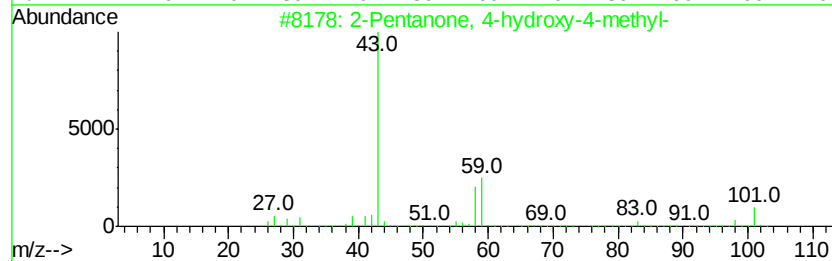
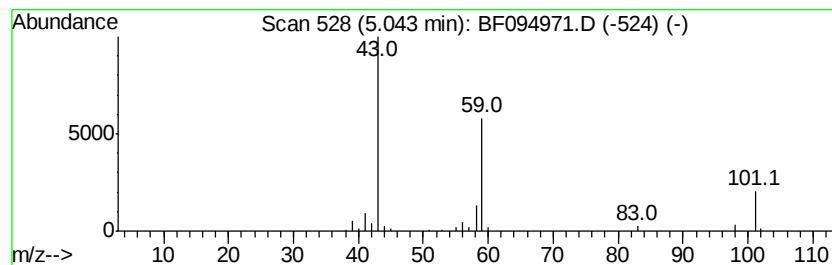
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.04 | 10.73 ng | 324451 | 1,4-Dichlorobenzene-d4 | 7.72 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2 | 000123-42-2 | 64   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2 | 000540-88-5 | 39   |
| 3    |    | 3-Hexanol                           | 102 | C6H14O  | 000623-37-0 | 28   |
| 4    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2 | 000057-71-6 | 9    |
| 5    |    | Butane, 1-ethoxy-                   | 102 | C6H14O  | 000628-81-9 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

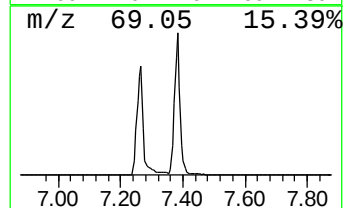
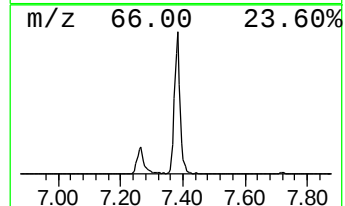
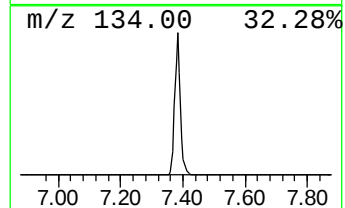
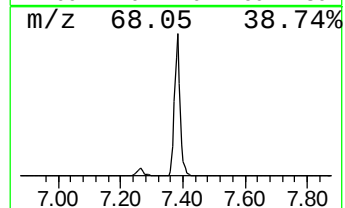
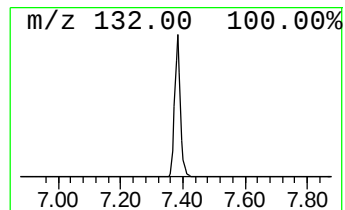
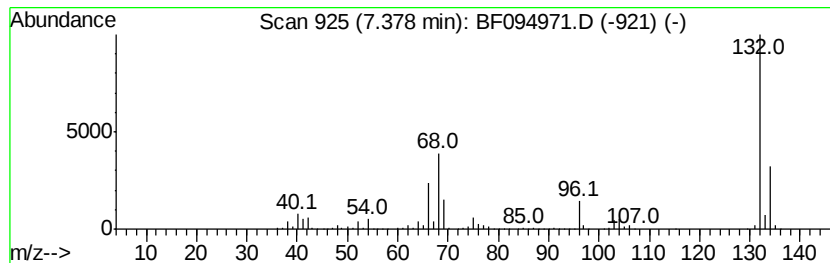
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown7.38 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.38 | 103.47 ng | 3129300 | 1,4-Dichlorobenzene-d4 | 7.72 |

| 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  | 27   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 10   |
| 5    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 9    |



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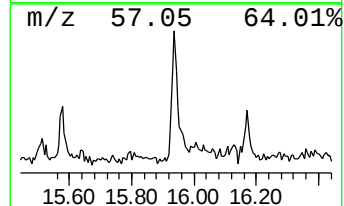
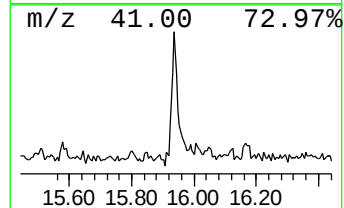
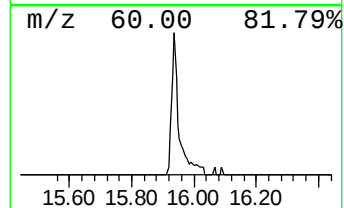
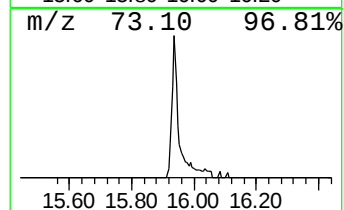
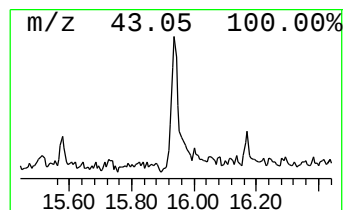
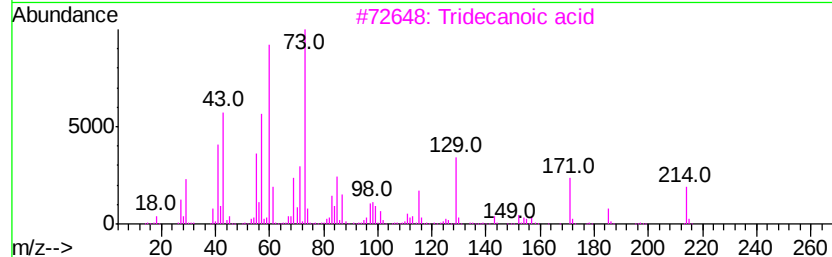
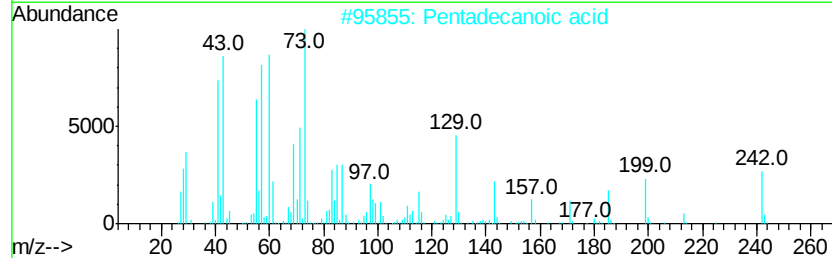
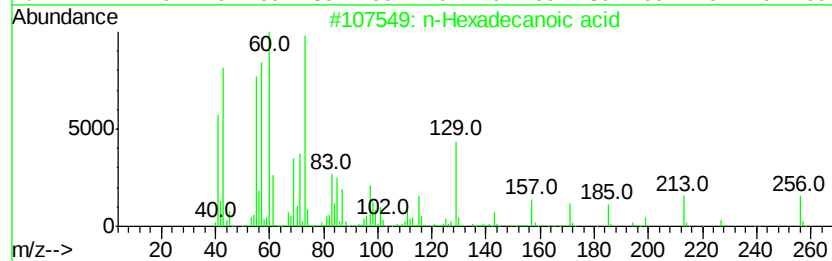
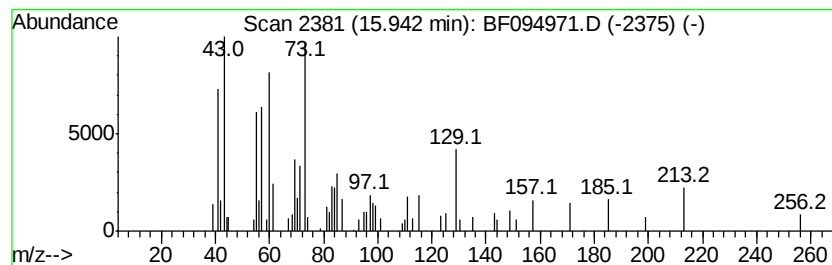
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD |  | R.T.  |
|-------|---------|--------|------------------|--|-------|
| 15.94 | 3.11 ng | 124020 | Phenanthrene-d10 |  | 14.97 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 87   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 64   |
| 4    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 64   |
| 5    |    |   | n-Decanoic acid     | 172 | C10H20O2 | 000334-48-5 | 52   |



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ALS Vial : 18 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-06-4.5-5.0

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF050217.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... | 5.04  | 10.7    | ng    | 324451   | 1                     | 7.72  | 604869 | 20.0 |
| unknown7.38          | 7.38  | 103.5   | ng    | 3129300  | 1                     | 7.72  | 604869 | 20.0 |
| n-Hexadecanoic acid  | 15.94 | 3.1     | ng    | 124020   | 4                     | 14.97 | 796539 | 20.0 |