

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\  
 Data File : BM010181.D  
 Acq On : 24 May 2017 15:27  
 Operator : SJ/MA  
 Sample : I3305-04  
 Misc :  
 ALS Vial : 11 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 DSK-SB2(10-11.8)

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\_M\METHODS\8270-BM051917.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         | 3.281       | 29            | 33          | 38           | rVB      | 92706          | 114865        | 1.35%           | 0.228%        |
| 2         | 5.069       | 333           | 337         | 348          | rVB      | 189466         | 269911        | 3.17%           | 0.536%        |
| 3         | 5.534       | 409           | 416         | 427          | rBV      | 2553180        | 3745753       | 43.99%          | 7.443%        |
| 4         | 7.139       | 681           | 689         | 699          | rBV      | 2331269        | 3634018       | 42.68%          | 7.220%        |
| 5         | 7.492       | 742           | 749         | 761          | rBV      | 2522107        | 3968807       | 46.61%          | 7.886%        |
| 6         | 7.951       | 820           | 827         | 833          | rBV      | 536370         | 855385        | 10.05%          | 1.700%        |
| 7         | 8.269       | 874           | 881         | 892          | rBV      | 1892914        | 3102370       | 36.44%          | 6.164%        |
| 8         | 9.139       | 1020          | 1029        | 1038         | rBV      | 1341184        | 2154780       | 25.31%          | 4.281%        |
| 9         | 10.757      | 1296          | 1304        | 1311         | rBV      | 609406         | 1043828       | 12.26%          | 2.074%        |
| 10        | 11.974      | 1504          | 1511        | 1514         | rBV4     | 59375          | 103796        | 1.22%           | 0.206%        |
| 11        | 12.439      | 1585          | 1590        | 1598         | rVB6     | 46316          | 104184        | 1.22%           | 0.207%        |
| 12        | 12.986      | 1679          | 1683        | 1688         | rVV5     | 86565          | 126318        | 1.48%           | 0.251%        |
| 13        | 13.204      | 1714          | 1720        | 1726         | rBV      | 3697758        | 5157540       | 60.57%          | 10.248%       |
| 14        | 13.321      | 1734          | 1740        | 1750         | rBV4     | 146128         | 381020        | 4.48%           | 0.757%        |
| 15        | 13.963      | 1844          | 1849        | 1857         | rVB      | 614920         | 887961        | 10.43%          | 1.764%        |
| 16        | 14.045      | 1858          | 1863        | 1867         | rBV      | 462332         | 669103        | 7.86%           | 1.329%        |
| 17        | 14.080      | 1867          | 1869        | 1873         | rVB2     | 84832          | 97344         | 1.14%           | 0.193%        |
| 18        | 14.286      | 1898          | 1904        | 1908         | rBV2     | 245466         | 413651        | 4.86%           | 0.822%        |
| 19        | 14.374      | 1914          | 1919        | 1924         | rVB      | 420943         | 601775        | 7.07%           | 1.196%        |
| 20        | 14.451      | 1928          | 1932        | 1935         | rVV5     | 74242          | 106522        | 1.25%           | 0.212%        |
| 21        | 14.515      | 1940          | 1943        | 1950         | rVB7     | 92869          | 159056        | 1.87%           | 0.316%        |
| 22        | 14.586      | 1950          | 1955        | 1962         | rBV2     | 818333         | 1341953       | 15.76%          | 2.666%        |
| 23        | 15.192      | 2056          | 2058        | 2064         | rVB5     | 90179          | 118081        | 1.39%           | 0.235%        |
| 24        | 15.262      | 2067          | 2070        | 2076         | rVB5     | 91806          | 156088        | 1.83%           | 0.310%        |
| 25        | 15.327      | 2077          | 2081        | 2085         | rBV3     | 169265         | 250214        | 2.94%           | 0.497%        |
| 26        | 16.074      | 2202          | 2208        | 2213         | rBV      | 3073164        | 4157135       | 48.83%          | 8.260%        |
| 27        | 17.327      | 2416          | 2421        | 2430         | rVB      | 1193374        | 1722386       | 20.23%          | 3.422%        |
| 28        | 18.174      | 2561          | 2565        | 2574         | rBV3     | 294730         | 476623        | 5.60%           | 0.947%        |
| 29        | 19.445      | 2777          | 2781        | 2786         | rVB3     | 128682         | 161802        | 1.90%           | 0.321%        |
| 30        | 19.927      | 2858          | 2863        | 2872         | rBV      | 6964057        | 8514336       | 100.00%         | 16.917%       |
| 31        | 21.486      | 3123          | 3128        | 3134         | rBV      | 2123250        | 2751238       | 32.31%          | 5.466%        |
| 32        | 23.850      | 3524          | 3530        | 3538         | rVB      | 1515054        | 2981355       | 35.02%          | 5.924%        |

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ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

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\_M\METHODS\8270-BM051917.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

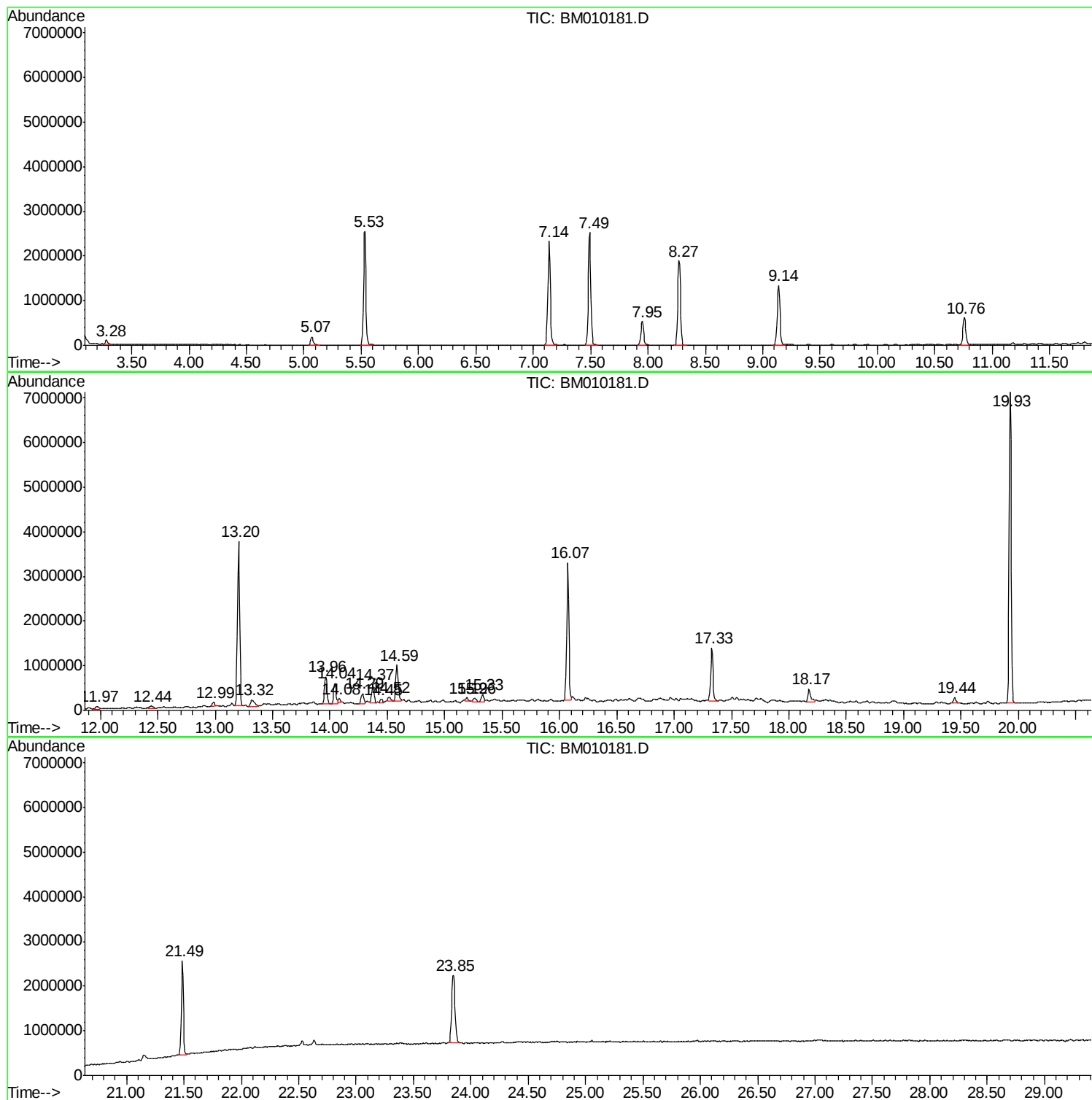
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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DSK-SB2(10-11.8)

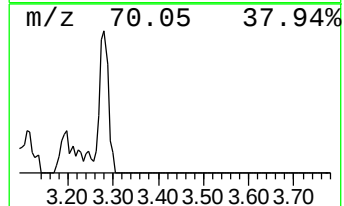
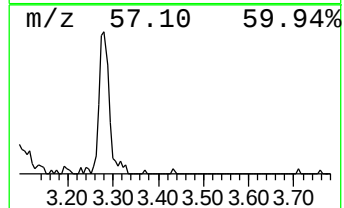
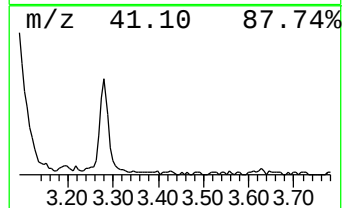
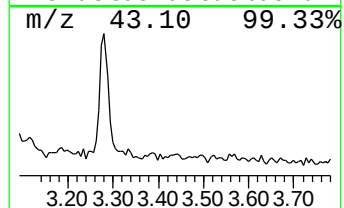
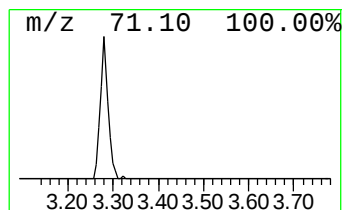
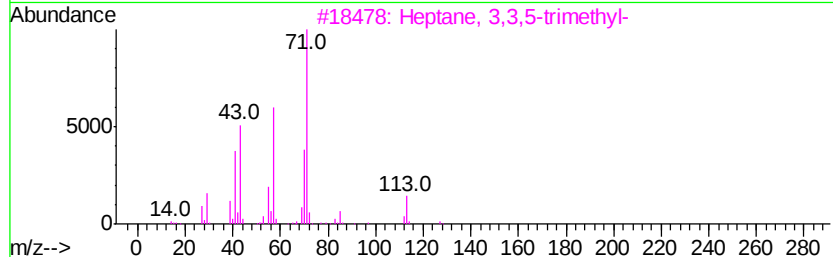
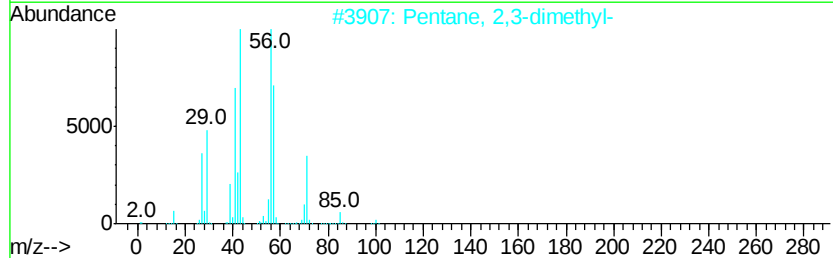
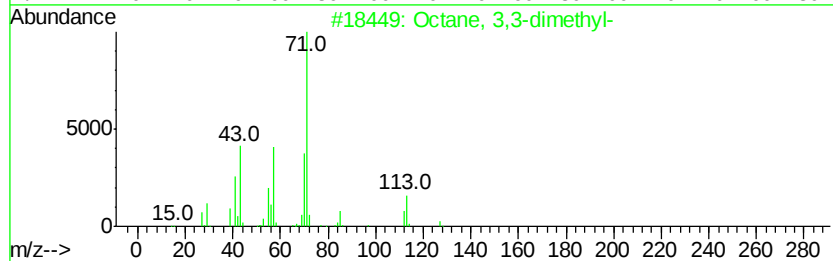
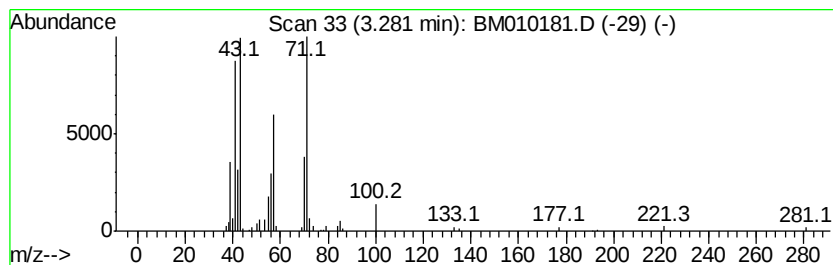
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 Octane, 3,3-dimethyl- Concentration Rank 10

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 3.28 | 2.69 ng | 114865 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# | of | 5 | Tentative ID              | MW  | MolForm | CAS#        | Qual |
|------|----|---|---------------------------|-----|---------|-------------|------|
| 1    |    |   | Octane, 3,3-dimethyl-     | 142 | C10H22  | 004110-44-5 | 59   |
| 2    |    |   | Pentane, 2,3-dimethyl-    | 100 | C7H16   | 000565-59-3 | 59   |
| 3    |    |   | Heptane, 3,3,5-trimethyl- | 142 | C10H22  | 007154-80-5 | 59   |
| 4    |    |   | Heptane                   | 100 | C7H16   | 000142-82-5 | 53   |
| 5    |    |   | 3-Hexanone, 4,4-dimethyl- | 128 | C8H16O  | 019550-14-2 | 50   |



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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

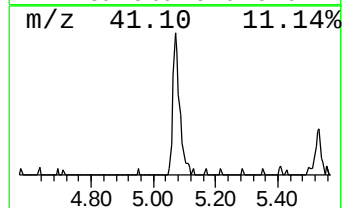
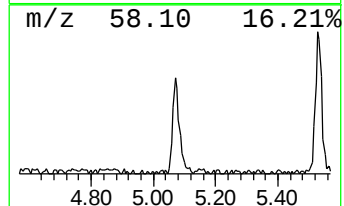
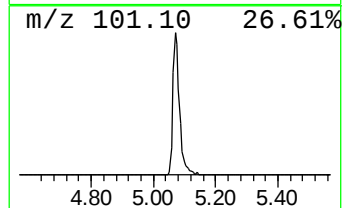
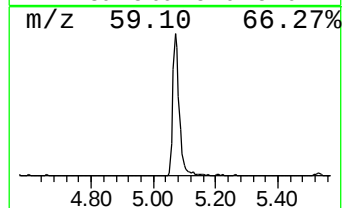
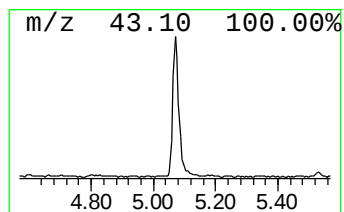
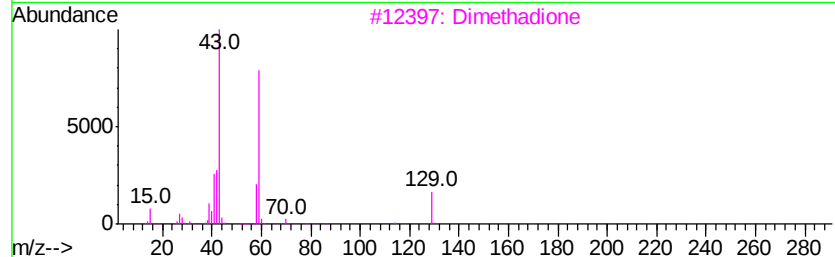
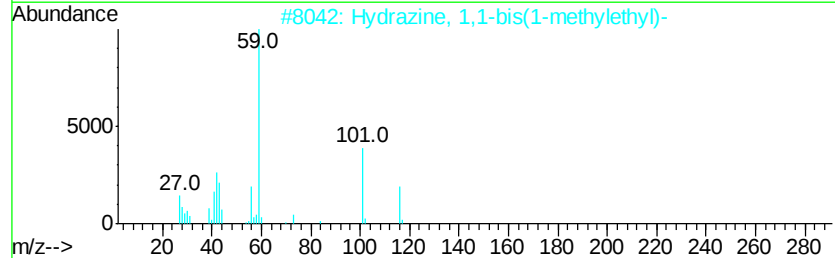
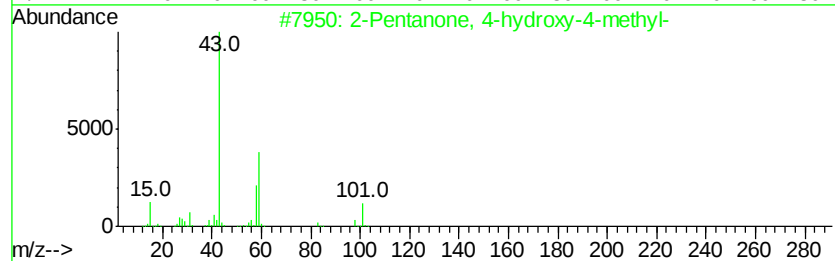
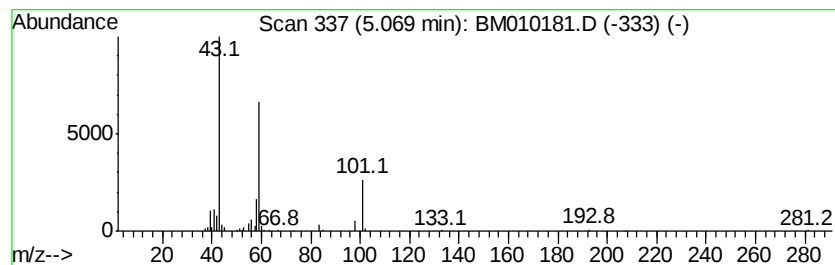
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.07 | 6.31 ng | 269911 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# | of | Tentative ID                       | MW  | MolForm | CAS#        | Qual |
|------|----|------------------------------------|-----|---------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-   | 116 | C6H12O2 | 000123-42-2 | 50   |
| 2    |    | Hydrazine, 1,1-bis(1-methylethyl)- | 116 | C6H16N2 | 000921-14-2 | 47   |
| 3    |    | Dimethadione                       | 129 | C5H7NO3 | 000695-53-4 | 33   |
| 4    |    | 2,3-Butanedione, monooxime         | 101 | C4H7NO2 | 000057-71-6 | 25   |
| 5    |    | Butyl aldoxime, 3-methyl-, syn-    | 101 | C5H11NO | 005780-40-5 | 25   |



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Misc :  
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Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

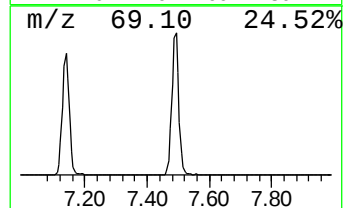
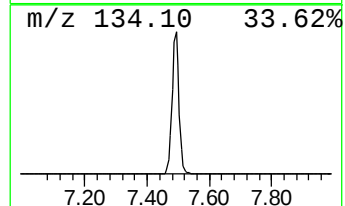
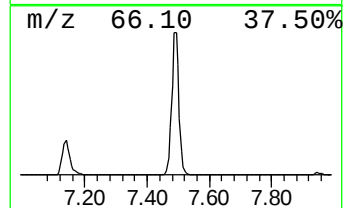
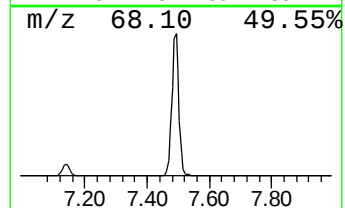
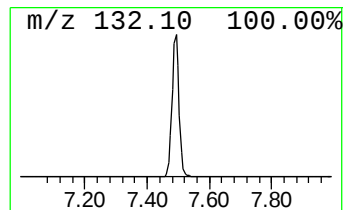
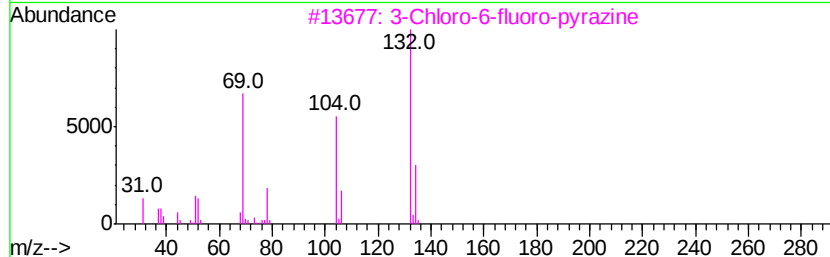
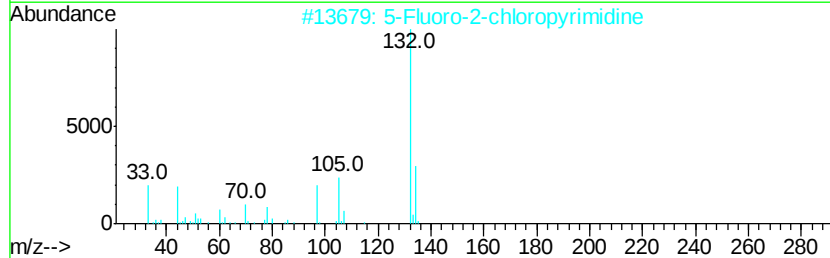
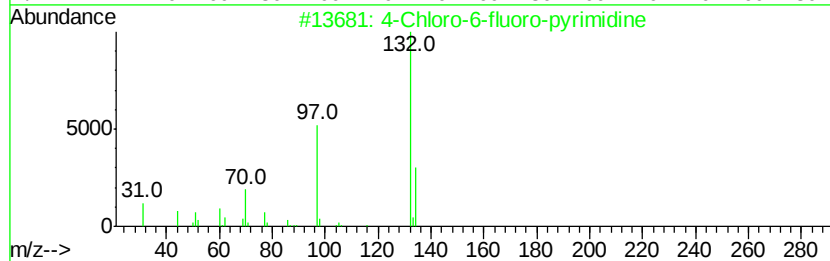
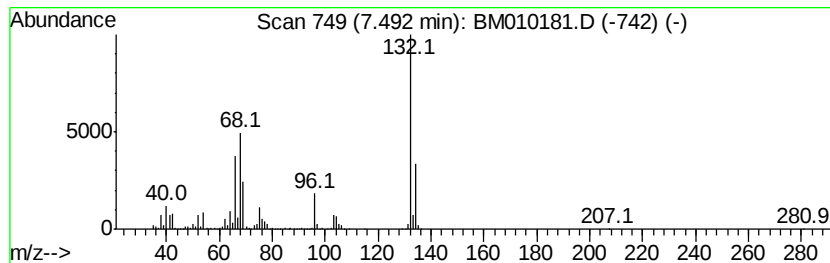
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown7.49 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.49 | 92.80 ng | 3968810 | 1,4-Dichlorobenzene-d4 | 7.95 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 4-Chloro-6-fluoro-pyrimidine     | 132 | C4H2ClFN2 | 051422-01-6  | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine      | 132 | C4H2ClFN2 | 062802-42-0  | 27   |
| 3    |    | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 4    |    | 1H-Benzimidazole, 2-methyl-      | 132 | C8H8N2    | 000615-15-6  | 27   |
| 5    |    | 1,3-Cyclopentanedione, 2-chloro- | 132 | C5H5ClO2  | 014203-19-1  | 25   |



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ALS Vial : 11 Sample Multiplier: 1

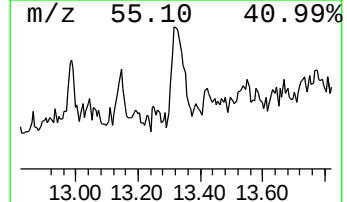
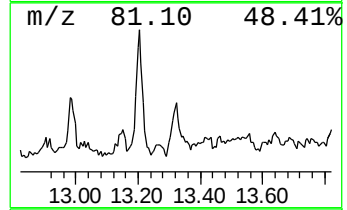
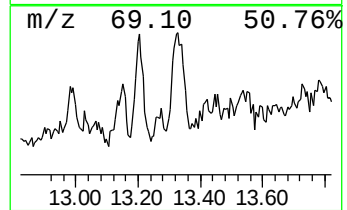
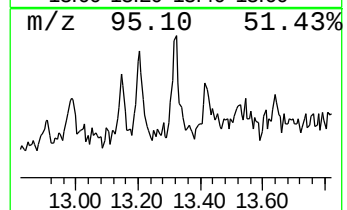
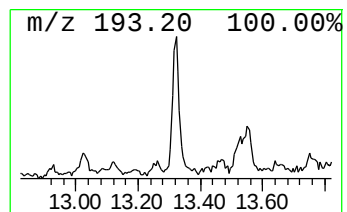
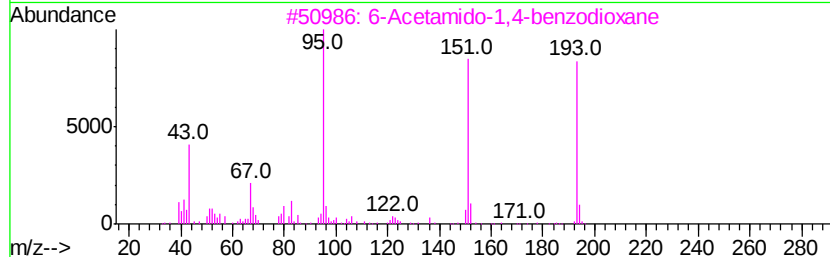
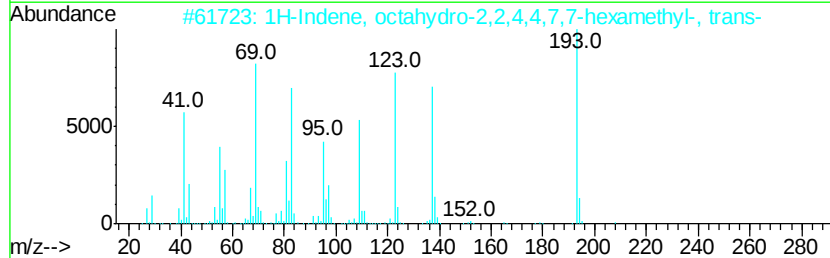
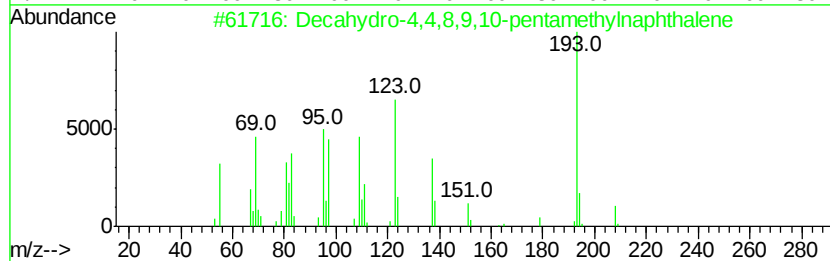
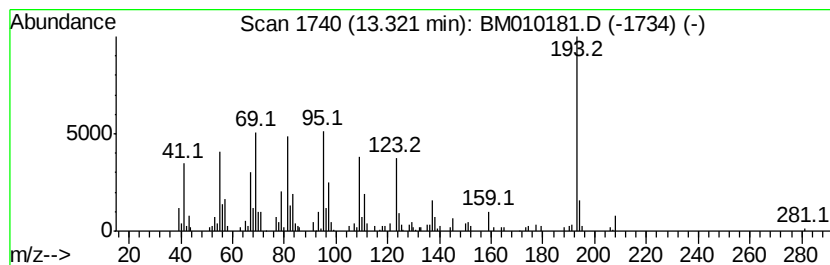
Instrument :  
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DSK-SB2(10-11.8)

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

\*\*\*\*\*  
Peak Number 5 Decahydro-4,4,8,9,10-pentam... Concentration Rank 7

| R.T.    | EstConc | Area                                | Relative to ISTD | R.T.           |
|---------|---------|-------------------------------------|------------------|----------------|
| 13.32   | 5.68 ng | 381020                              | Acenaphthene-d10 | 14.58          |
| Hit# of | 5       | Tentative ID                        | MW MolForm       | CAS# Qual      |
| 1       |         | Decahydro-4,4,8,9,10-pentamethyl... | 208 C15H28       | 080655-44-3 90 |
| 2       |         | 1H-Indene, octahydro-2,2,4,4,7,7... | 208 C15H28       | 054832-83-6 53 |
| 3       |         | 6-Acetamido-1,4-benzodioxane        | 193 C10H11N03    | 063546-19-0 43 |
| 4       |         | 2-Anthracenamine                    | 193 C14H11N      | 000613-13-8 35 |
| 5       |         | Pyrimido(5,4-e)-as-triazine-5,7(... | 193 C7H7N5O2     | 000084-82-2 35 |



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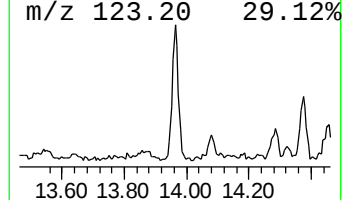
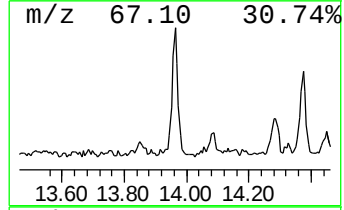
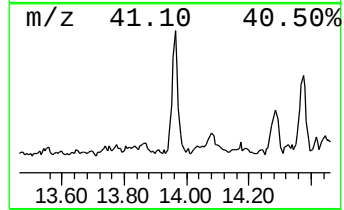
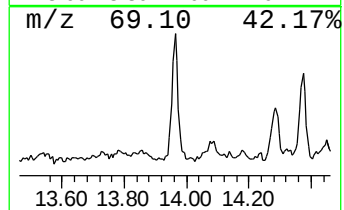
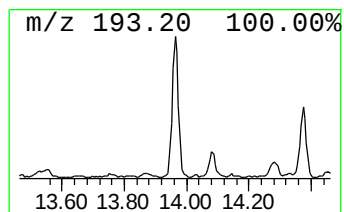
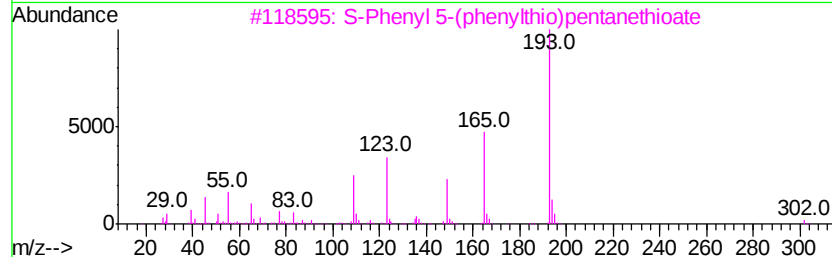
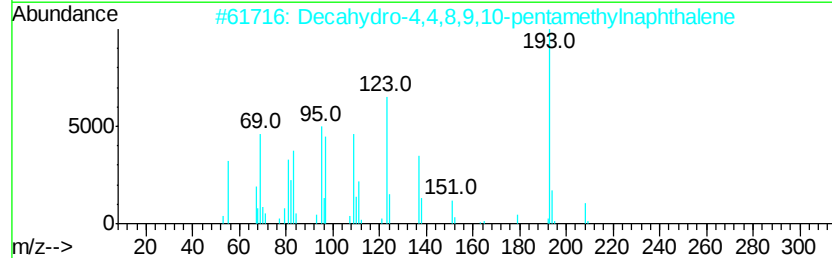
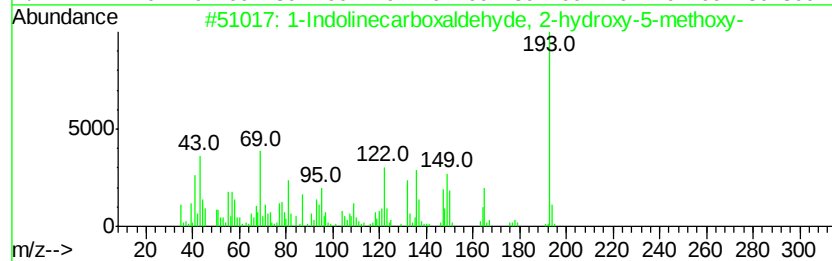
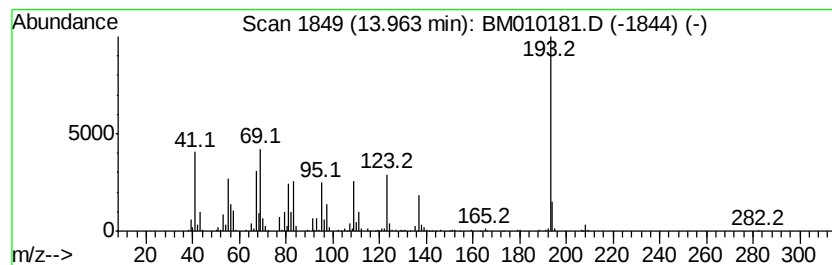
Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 6 1-Indolinecarboxaldehyde, 2... Concentration Rank 3

| R.T.    | EstConc  | Area                                | Relative to ISTD | R.T.            |
|---------|----------|-------------------------------------|------------------|-----------------|
| 13.96   | 13.23 ng | 887961                              | Acenaphthene-d10 | 14.58           |
| Hit# of | 5        | Tentative ID                        | MW MolForm       | CAS# Qual       |
| 1       |          | 1-Indolinecarboxaldehyde, 2-hydr... | 193 C10H11N03    | 013303-70-3 47  |
| 2       |          | Decahydro-4,4,8,9,10-pentamethyl... | 208 C15H28       | 080655-44-3 42  |
| 3       |          | S-Phenyl 5-(phenylthio)pentaneth... | 302 C17H18S2     | 1000234-40-7 38 |
| 4       |          | Iminostilbene                       | 193 C14H11N      | 000256-96-2 35  |
| 5       |          | 2-Anthracenamine                    | 193 C14H11N      | 000613-13-8 35  |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\  
Data File : BM010181.D  
Acq On : 24 May 2017 15:27  
Operator : SJ/MA  
Sample : I3305-04  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

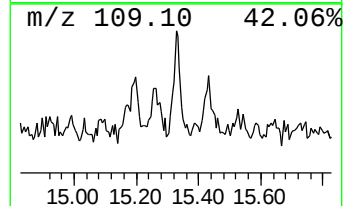
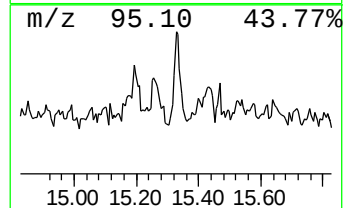
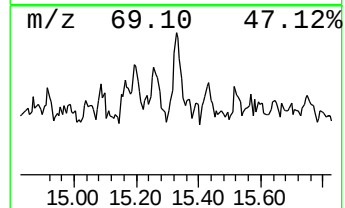
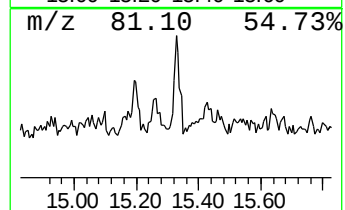
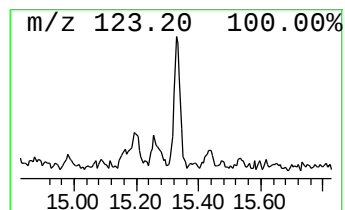
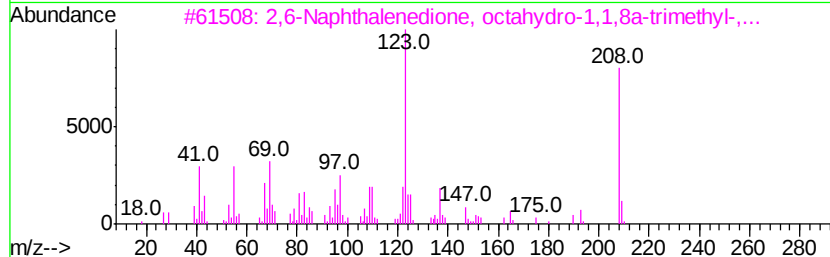
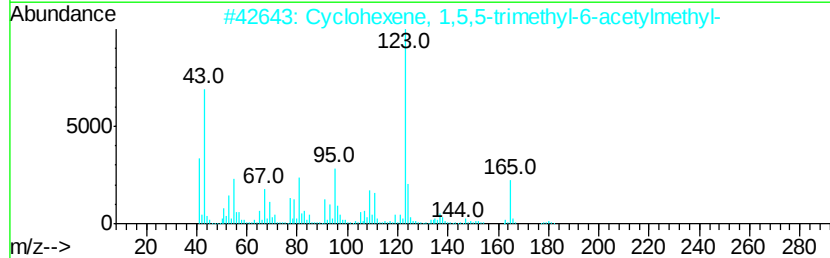
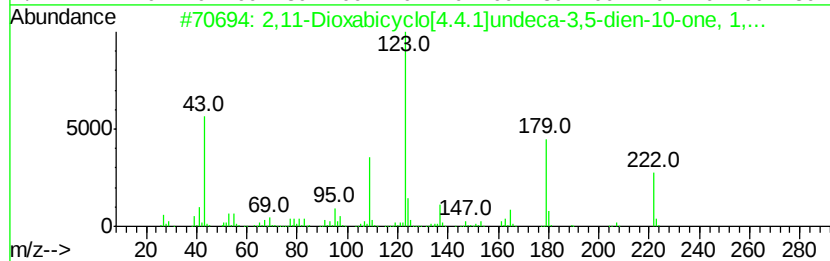
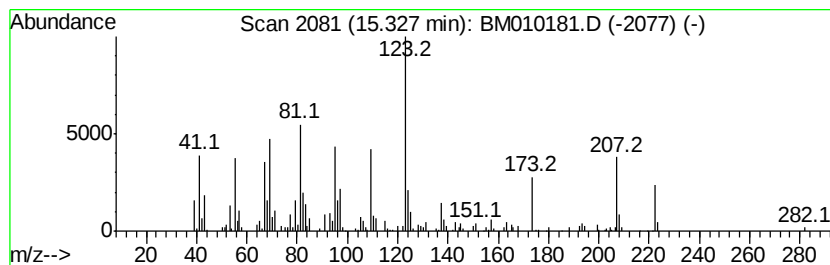
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 11 unknown15.33 Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.33 | 3.73 ng | 250214 | Acenaphthene-d10 | 14.58 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2,11-Dioxabicyclo[4.4.1]undeca-3... | 222 | C13H18O3     | 070412-52-1 | 49      |      |      |
| 2    | Cyclohexene, 1,5,5-trimethyl-6-a... | 180 | C12H20O      | 211563-96-1 | 47      |      |      |
| 3    | 2,6-Naphthalenedione, octahydro-... | 208 | C13H20O2     | 057289-16-4 | 38      |      |      |
| 4    | Magnesium, bis(acetylacetonate)     | 222 | C10H14MgO4   | 068488-07-3 | 38      |      |      |
| 5    | Bicyclo[4.1.0]heptane-7-carboxam... | 222 | C11H14N2O5   | 329912-72-3 | 38      |      |      |



Data Path : Z:\HPCHEM1\BNA M\DATA\BM052417\  
Data File : BM010181.D  
Acq On : 24 May 2017 15:27  
Operator : SJ/MA  
Sample : I3305-04  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

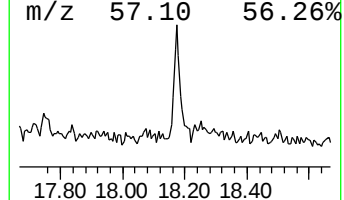
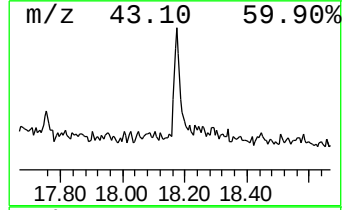
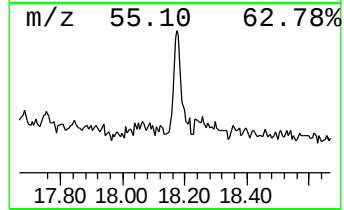
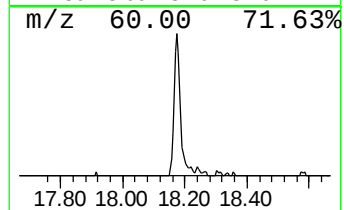
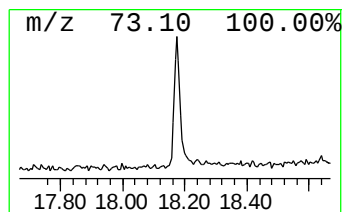
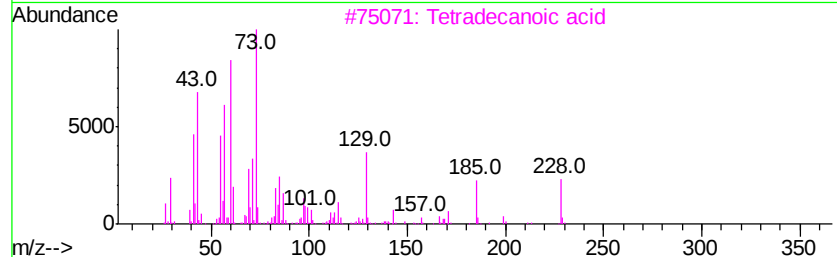
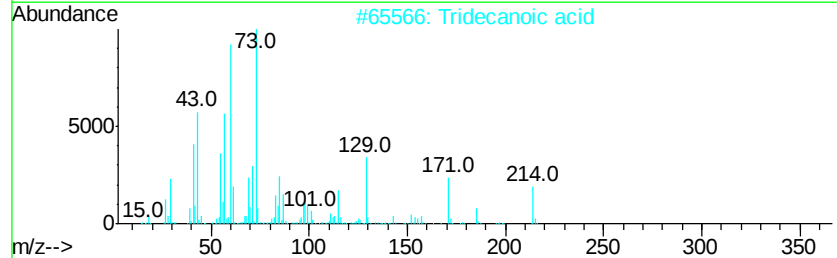
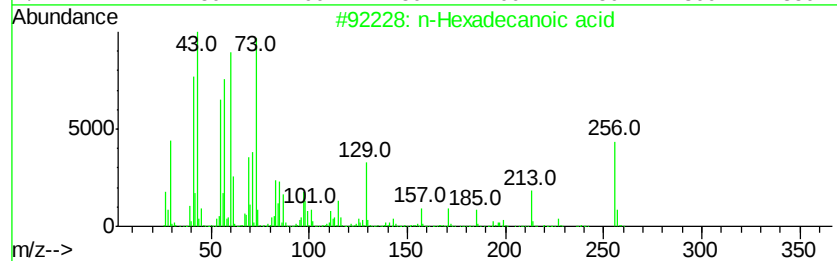
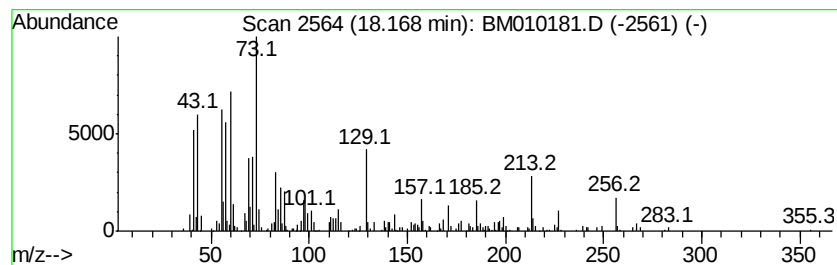
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 12 n-Hexadecanoic acid Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.17 | 5.53 ng | 476623 | Phenanthrene-d10 | 17.33 |

| Hit# | of | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---------------------|-----|----------|-------------|------|
| 1    | 5  | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 95   |
| 2    |    | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 90   |
| 3    |    | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 53   |
| 4    |    | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 49   |
| 5    |    | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 49   |



Data Path : Z:\HPCHEM1\BNA\_M\DATA\BM052417\  
Data File : BM010181.D  
Acq On : 24 May 2017 15:27  
Operator : SJ/MA  
Sample : I3305-04  
Misc :  
ALS Vial : 11 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
DSK-SB2(10-11.8)

Quant Method : Z:\HPCHEM1\BNA\_M\METHODS\8270-BM051917.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 |
| Octane, 3,3-dimet... | 3.28  | 2.7     | ng    | 114865   | 1                     | 7.95  | 855385  | 20.0 |
| 2-Pentanone, 4-hy... | 5.07  | 6.3     | ng    | 269911   | 1                     | 7.95  | 855385  | 20.0 |
| unknown7.49          | 7.49  | 92.8    | ng    | 3968810  | 1                     | 7.95  | 855385  | 20.0 |
| Decahydro-4,4,8,9... | 13.32 | 5.7     | ng    | 381020   | 3                     | 14.58 | 1341950 | 20.0 |
| 1-Indolinecarboxa... | 13.96 | 13.2    | ng    | 887961   | 3                     | 14.58 | 1341950 | 20.0 |
| unknown15.33         | 15.33 | 3.7     | ng    | 250214   | 3                     | 14.58 | 1341950 | 20.0 |
| n-Hexadecanoic acid  | 18.17 | 5.5     | ng    | 476623   | 4                     | 17.33 | 1722390 | 20.0 |