

Data Path : Z:\HPCHEM1\BNA M\DATA\BM051217\  
 Data File : BM010028.D  
 Acq On : 12 May 2017 17:51  
 Operator : SJ/MA  
 Sample : I3098-06  
 Misc :  
 ALS Vial : 9 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 MW-5

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-BM051117.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         | 4.893       | 303           | 307         | 317          | rBV      | 121234         | 181651        | 2.82%           | 0.620%        |
| 2         | 5.351       | 378           | 385         | 393          | rBV      | 937541         | 1454029       | 22.56%          | 4.966%        |
| 3         | 6.940       | 650           | 655         | 669          | rBV      | 617970         | 1063823       | 16.51%          | 3.633%        |
| 4         | 7.293       | 709           | 715         | 728          | rBV      | 1687075        | 2652662       | 41.16%          | 9.060%        |
| 5         | 7.757       | 788           | 794         | 802          | rBV      | 288670         | 478637        | 7.43%           | 1.635%        |
| 6         | 8.075       | 841           | 848         | 857          | rBV      | 1355088        | 2181028       | 33.84%          | 7.449%        |
| 7         | 8.934       | 985           | 994         | 1007         | rBV      | 1292859        | 2183734       | 33.88%          | 7.458%        |
| 8         | 10.557      | 1261          | 1270        | 1280         | rBV      | 363395         | 659421        | 10.23%          | 2.252%        |
| 9         | 13.022      | 1682          | 1689        | 1701         | rBV      | 2755128        | 4040342       | 62.69%          | 13.799%       |
| 10        | 13.880      | 1830          | 1835        | 1841         | rBV2     | 54102          | 83934         | 1.30%           | 0.287%        |
| 11        | 14.416      | 1919          | 1926        | 1934         | rBV3     | 513542         | 814158        | 12.63%          | 2.781%        |
| 12        | 15.915      | 2174          | 2181        | 2198         | rBV      | 2338855        | 3416629       | 53.01%          | 11.669%       |
| 13        | 17.168      | 2388          | 2394        | 2404         | rBV      | 701644         | 1032738       | 16.02%          | 3.527%        |
| 14        | 18.045      | 2536          | 2543        | 2549         | rBV3     | 80888          | 118801        | 1.84%           | 0.406%        |
| 15        | 19.327      | 2757          | 2761        | 2765         | rBV2     | 80202          | 107495        | 1.67%           | 0.367%        |
| 16        | 19.792      | 2834          | 2840        | 2848         | rVB      | 5368124        | 6445141       | 100.00%         | 22.012%       |
| 17        | 21.045      | 3050          | 3053        | 3057         | rBV5     | 64343          | 72599         | 1.13%           | 0.248%        |
| 18        | 21.356      | 3101          | 3106        | 3113         | rBV      | 962452         | 1254676       | 19.47%          | 4.285%        |
| 19        | 22.503      | 3299          | 3301        | 3306         | rVB3     | 77822          | 91057         | 1.41%           | 0.311%        |
| 20        | 23.650      | 3490          | 3496        | 3504         | rVB      | 489198         | 947843        | 14.71%          | 3.237%        |

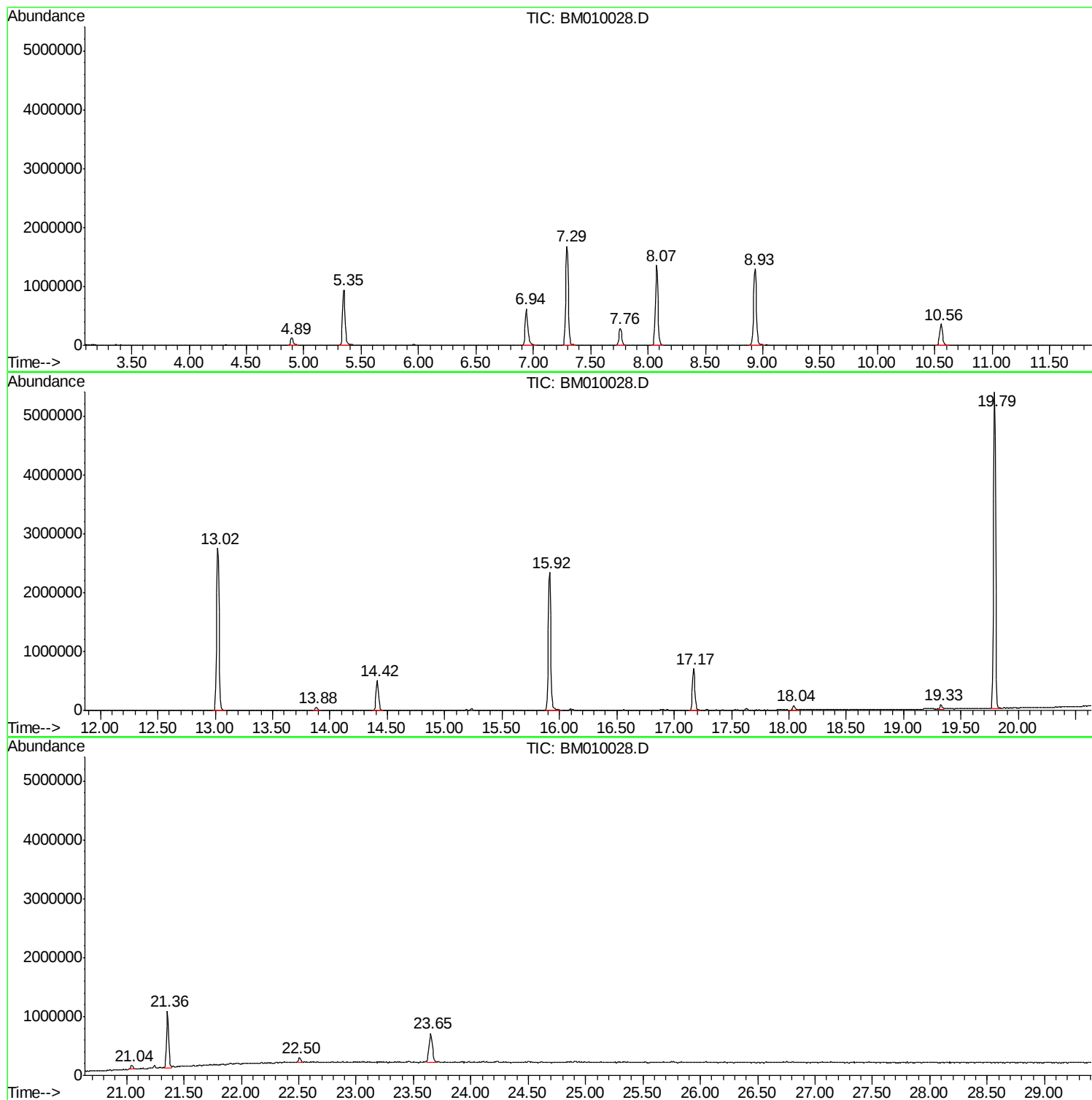
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BNA\_M  
ClientSampleId :  
MW-5

Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051117.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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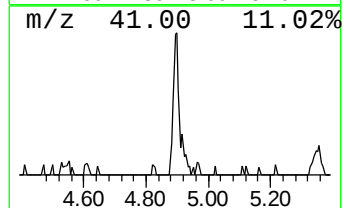
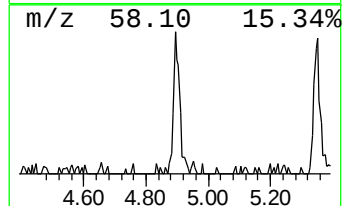
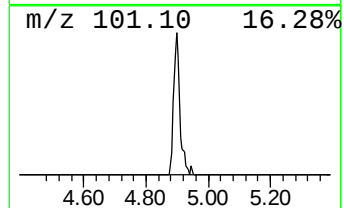
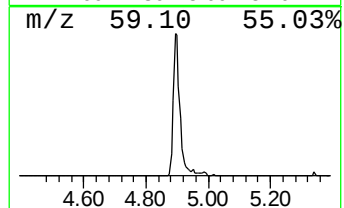
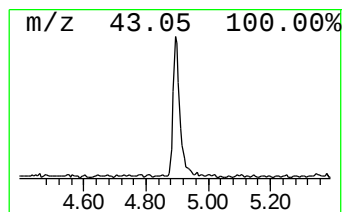
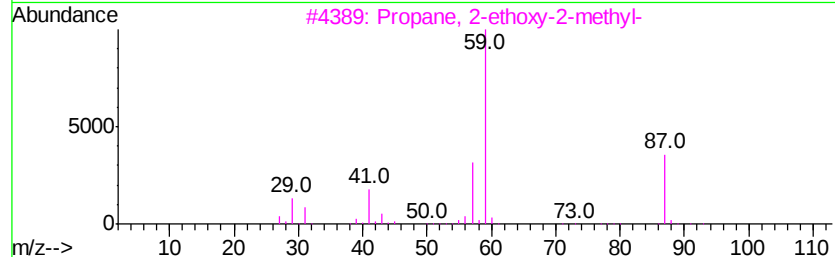
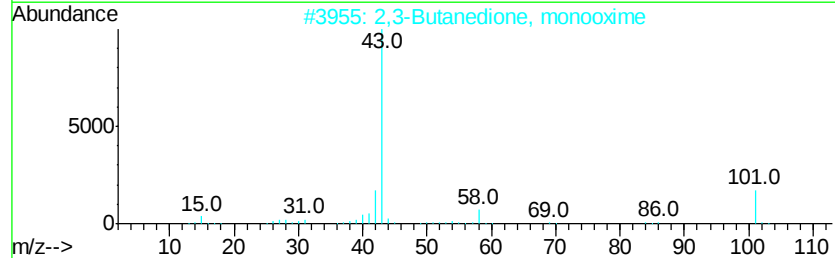
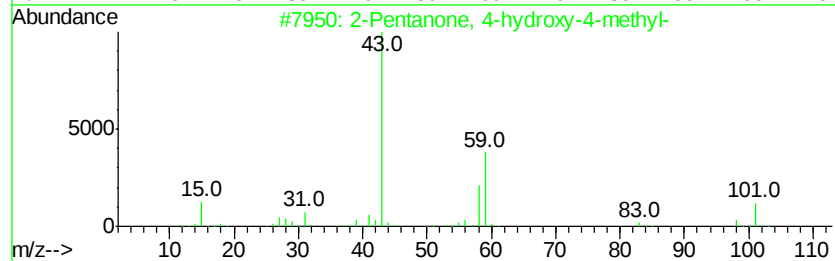
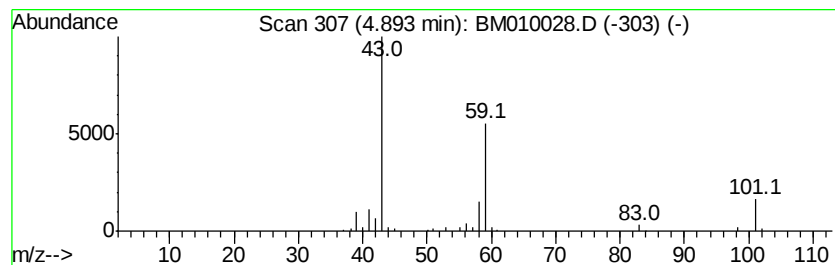
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.89 | 7.59 ng | 181651 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# of | 5                                | Tentative ID | MW      | MolForm     | CAS# | Qual |
|---------|----------------------------------|--------------|---------|-------------|------|------|
| 1       | 2-Pentanone, 4-hydroxy-4-methyl- | 116          | C6H12O2 | 000123-42-2 | 72   |      |
| 2       | 2,3-Butanedione, monooxime       | 101          | C4H7NO2 | 000057-71-6 | 9    |      |
| 3       | Propane, 2-ethoxy-2-methyl-      | 102          | C6H14O  | 000637-92-3 | 9    |      |
| 4       | Acetic acid, 2-propenyl ester    | 100          | C5H8O2  | 000591-87-7 | 9    |      |
| 5       | 1-Butene, 4-ethoxy-              | 100          | C6H12O  | 044611-46-3 | 9    |      |



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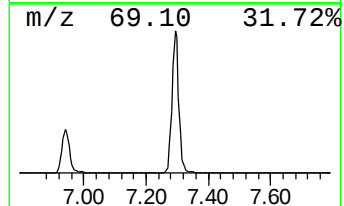
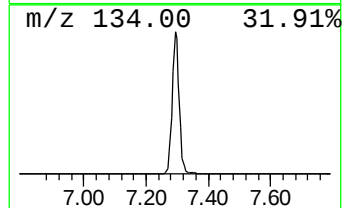
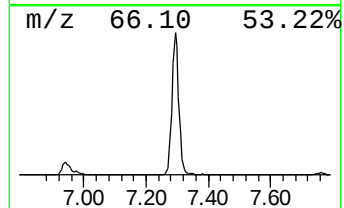
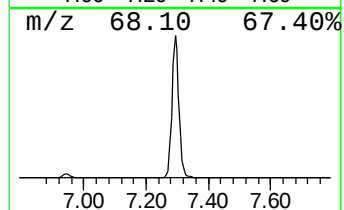
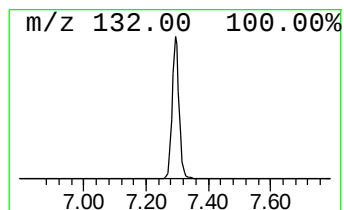
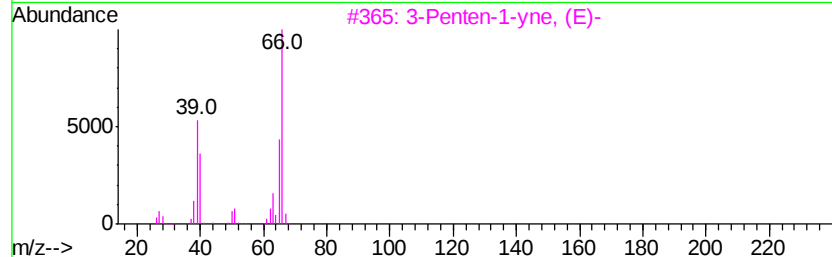
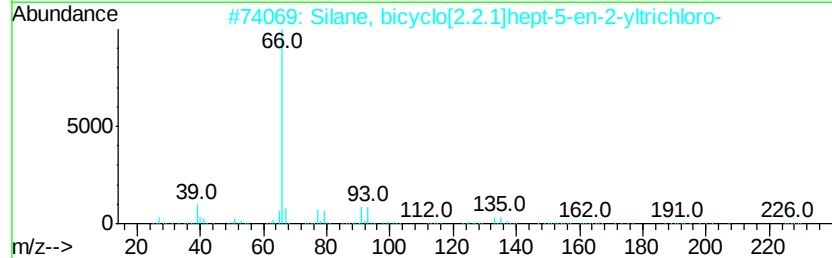
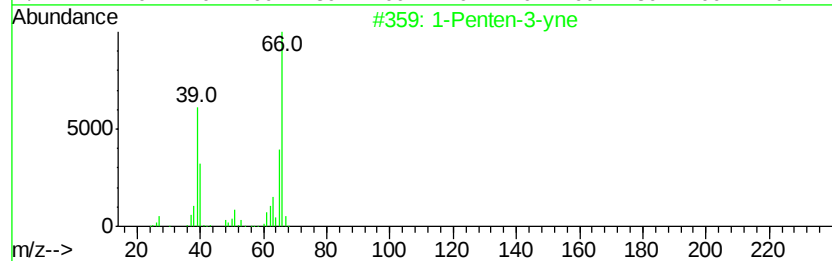
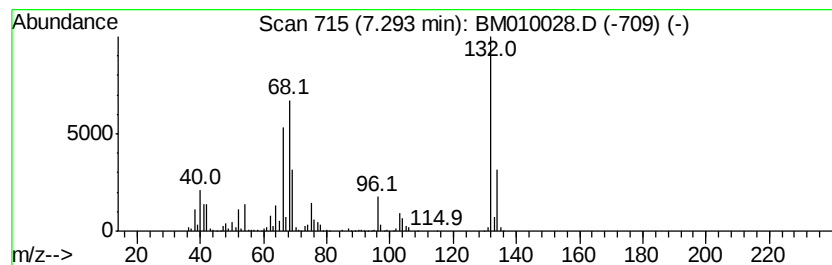
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Peak Number 2 unknown7.29 Concentration Rank 1

| R.T. | EstConc   | Area    | Relative to ISTD       | R.T. |
|------|-----------|---------|------------------------|------|
| 7.29 | 110.84 ng | 2652660 | 1,4-Dichlorobenzene-d4 | 7.76 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|-------------------------------------|-----|-----------|-------------|------|
| 1    | 5  | 1-Penten-3-yne                      | 66  | C5H6      | 000646-05-9 | 38   |
| 2    |    | Silane, bicyclo[2.2.1]hept-5-en-... | 226 | C7H9Cl3Si | 014319-64-3 | 35   |
| 3    |    | 3-Penten-1-yne, (E)-                | 66  | C5H6      | 002004-69-5 | 35   |
| 4    |    | 1,3-Cyclopentadiene                 | 66  | C5H6      | 000542-92-7 | 35   |
| 5    |    | Propanedinitrile                    | 66  | C3H2N2    | 000109-77-3 | 25   |



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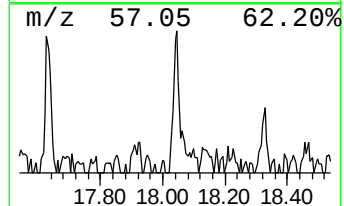
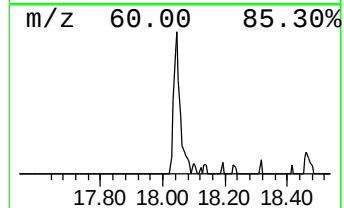
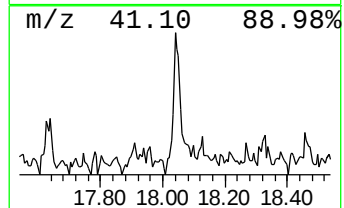
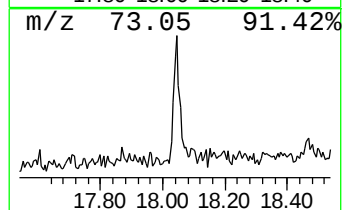
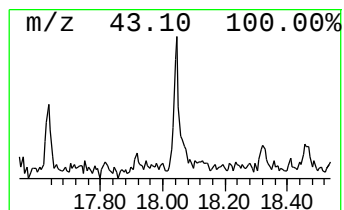
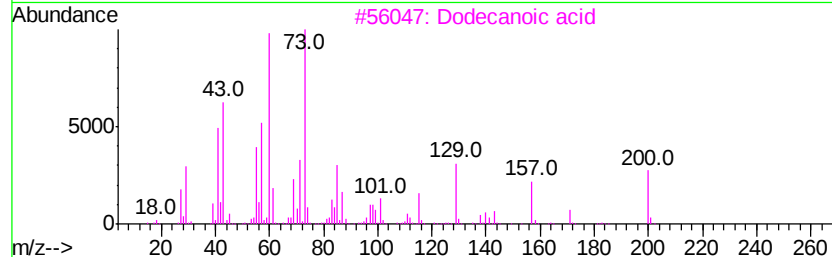
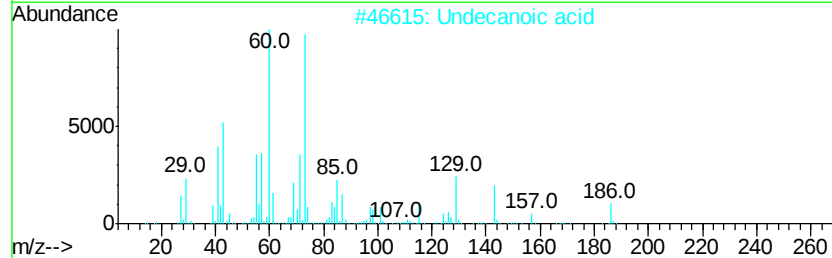
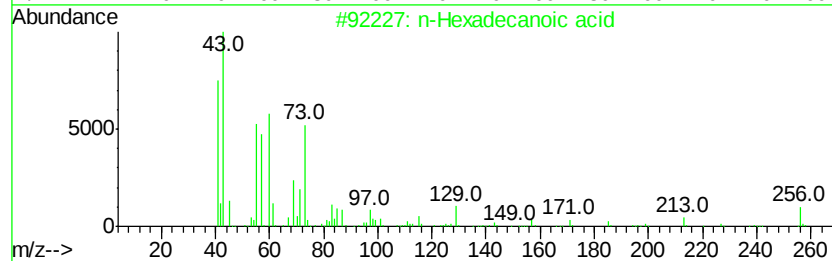
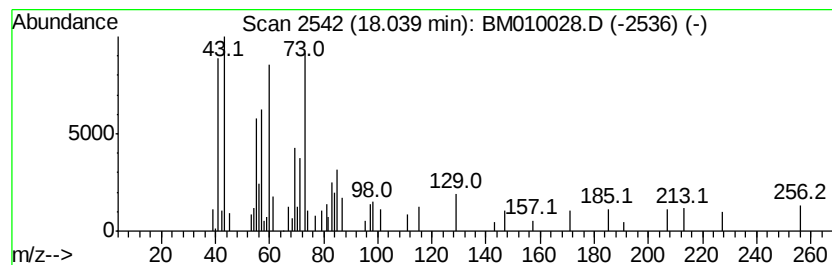
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.04 | 2.30 ng | 118801 | Phenanthrene-d10 | 17.17 |

| Hit# of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|---------|---|---------------------|-----|----------|-------------|------|
| 1       |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 98   |
| 2       |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 80   |
| 3       |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 80   |
| 4       |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 72   |
| 5       |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 58   |



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TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 4.89  | 7.6     | ng    | 181651   | 1                     | 7.76  | 478637  | 20.0 |
| unknown7.29          | 7.29  | 110.8   | ng    | 2652660  | 1                     | 7.76  | 478637  | 20.0 |
| n-Hexadecanoic acid  | 18.04 | 2.3     | ng    | 118801   | 4                     | 17.17 | 1032740 | 20.0 |