

Data Path : Z:\SVOASRV\HPCHEM1\BNA M\DATA\BM090418\  
 Data File : BM016659.D  
 Acq On : 04 Sep 2018 22:55  
 Operator : SJ/JU  
 Sample : J4759-05  
 Misc :  
 ALS Vial : 18 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 083018-DBRI-F-D-B

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:\SVOASRV\HPCHEM1\BNA\_M\METHODS\8270-BM082118.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         | 5.546       | 379           | 384         | 399          | rBV      | 292803         | 582856        | 7.42%           | 2.086%        |
| 2         | 7.181       | 657           | 662         | 676          | rBV      | 179382         | 365102        | 4.65%           | 1.306%        |
| 3         | 7.522       | 714           | 720         | 734          | rBV      | 816107         | 1426745       | 18.17%          | 5.105%        |
| 4         | 7.998       | 794           | 801         | 811          | rBV2     | 254750         | 490791        | 6.25%           | 1.756%        |
| 5         | 8.310       | 847           | 854         | 865          | rBV      | 1493842        | 2485777       | 31.65%          | 8.894%        |
| 6         | 9.181       | 996           | 1002        | 1022         | rBV      | 845946         | 1533430       | 19.53%          | 5.487%        |
| 7         | 10.798      | 1271          | 1277        | 1288         | rBV      | 286704         | 534751        | 6.81%           | 1.913%        |
| 8         | 13.251      | 1687          | 1694        | 1711         | rBV      | 3431140        | 4817410       | 61.35%          | 17.237%       |
| 9         | 14.104      | 1832          | 1839        | 1847         | rBV      | 84998          | 145011        | 1.85%           | 0.519%        |
| 10        | 14.633      | 1922          | 1929        | 1941         | rBV2     | 433847         | 719380        | 9.16%           | 2.574%        |
| 11        | 15.922      | 2144          | 2148        | 2155         | rBV      | 68325          | 88022         | 1.12%           | 0.315%        |
| 12        | 16.133      | 2178          | 2184        | 2202         | rBV      | 1714843        | 2831105       | 36.05%          | 10.130%       |
| 13        | 17.380      | 2390          | 2396        | 2407         | rBV      | 585310         | 946817        | 12.06%          | 3.388%        |
| 14        | 18.233      | 2536          | 2541        | 2547         | rBV4     | 69111          | 107651        | 1.37%           | 0.385%        |
| 15        | 19.968      | 2831          | 2836        | 2847         | rBV      | 7135816        | 7852932       | 100.00%         | 28.099%       |
| 16        | 21.527      | 3097          | 3101        | 3109         | rBV      | 1011995        | 1418037       | 18.06%          | 5.074%        |
| 17        | 23.803      | 3483          | 3488        | 3501         | rVB      | 784601         | 1601771       | 20.40%          | 5.731%        |

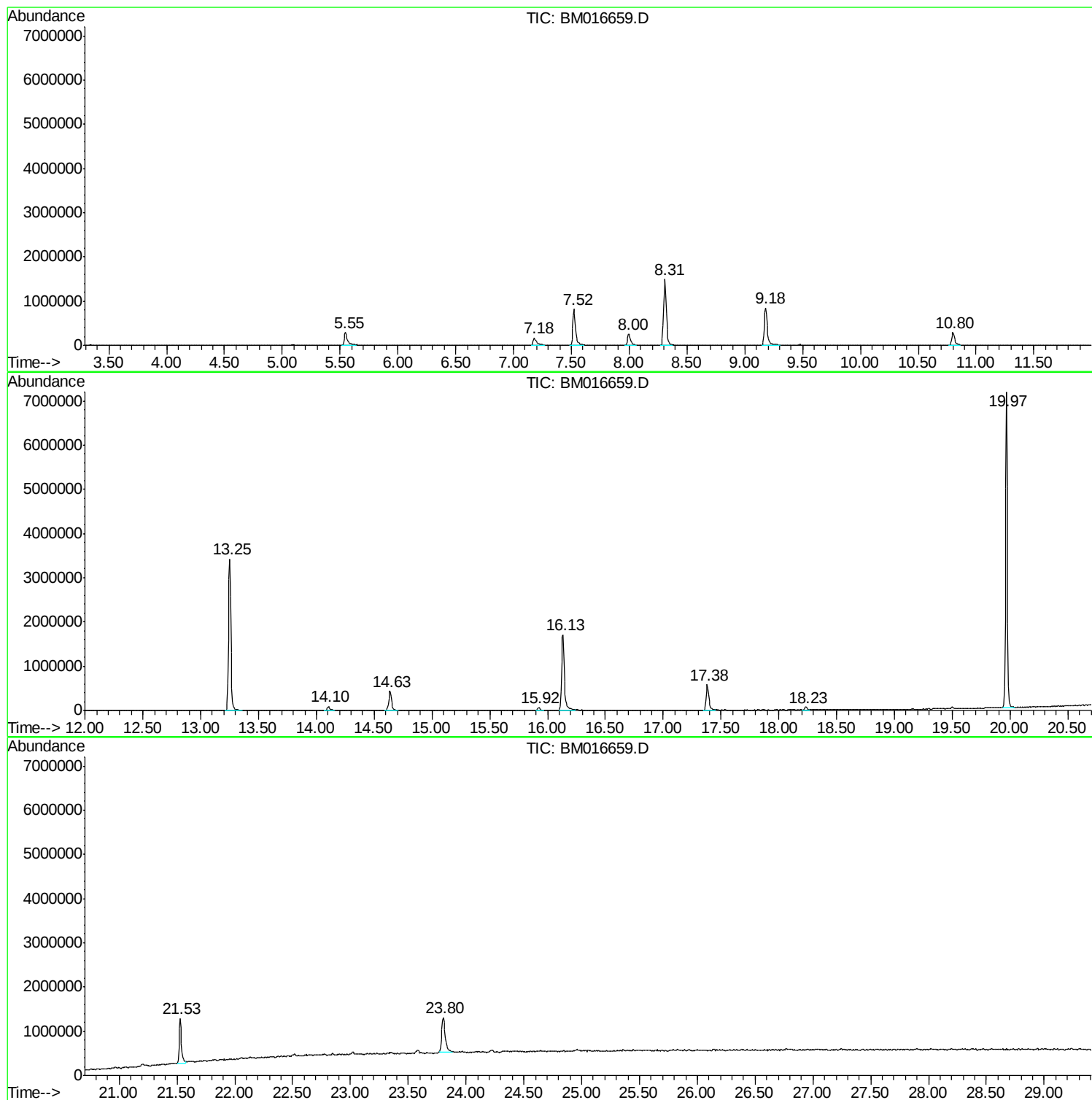
Sum of corrected areas: 27947588

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.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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Quant Method : Z:\SVOASRV\HPCHEM1\BNA M\METHODS\8270-BM082118.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

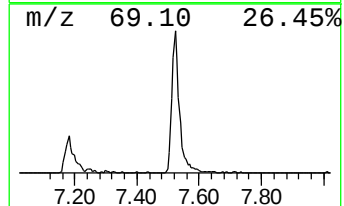
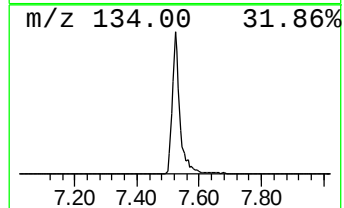
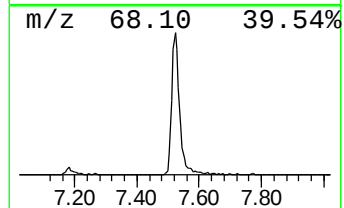
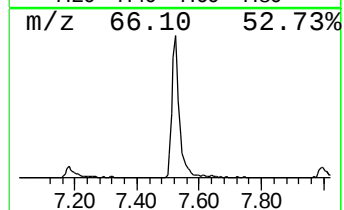
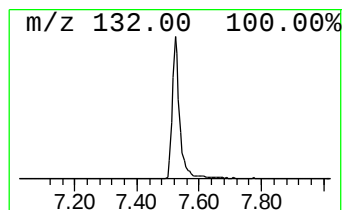
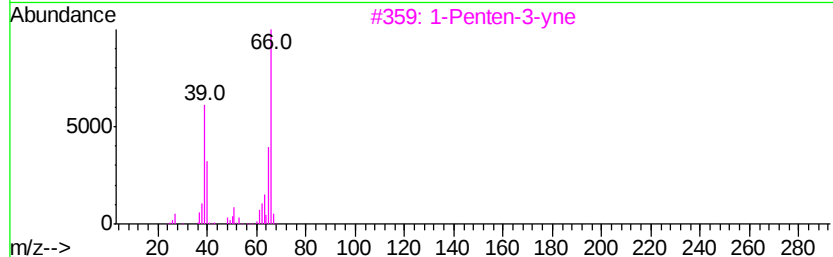
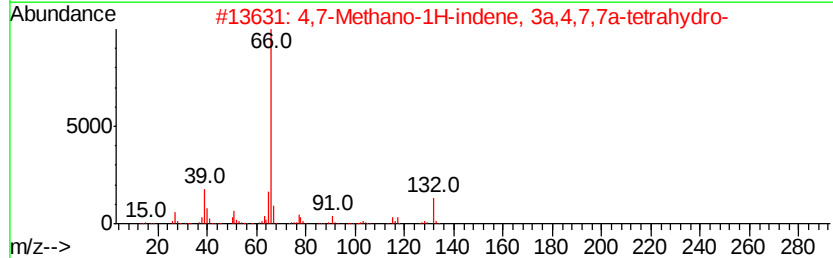
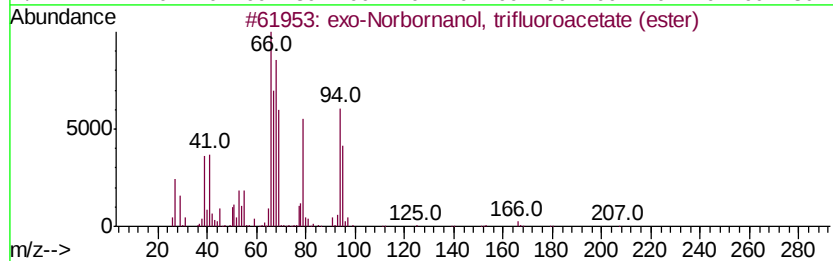
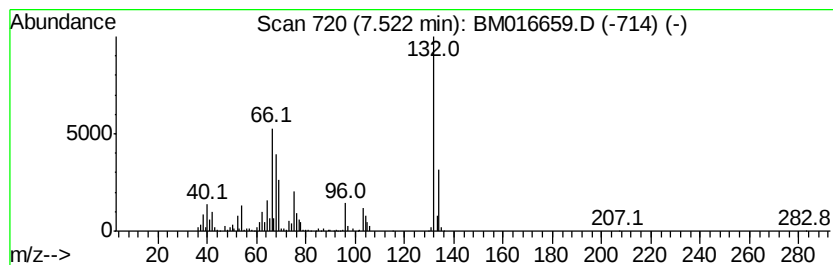
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 unknown7.52 Concentration Rank 2

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.52 | 58.14 ng | 1426750 | 1,4-Dichlorobenzene-d4 | 7.99 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | exo-Norbornanol, trifluoroacetat... | 208 | C9H11F3O2 | 1000245-87-9 | 32   |
| 2    |    | 4,7-Methano-1H-indene, 3a,4,7,7a... | 132 | C10H12    | 000077-73-6  | 28   |
| 3    |    | 1-Penten-3-yne                      | 66  | C5H6      | 000646-05-9  | 27   |
| 4    |    | 1,3-Cyclopentadiene                 | 66  | C5H6      | 000542-92-7  | 16   |
| 5    |    | Benzene, 1,3,5-trifluoro-           | 132 | C6H3F3    | 000372-38-3  | 14   |



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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

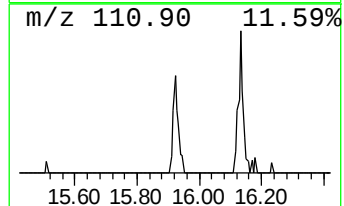
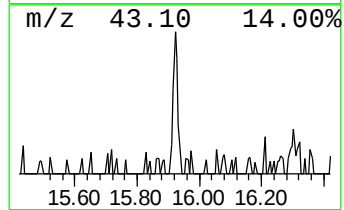
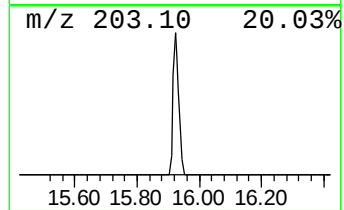
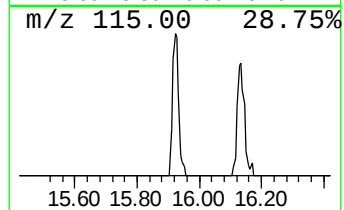
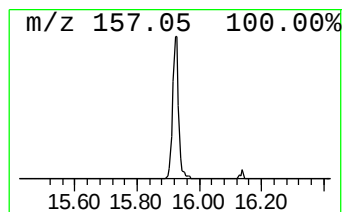
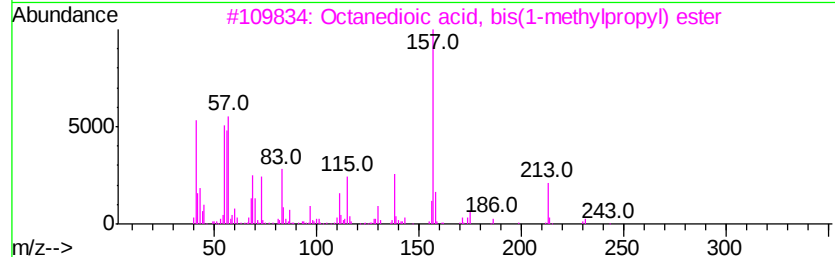
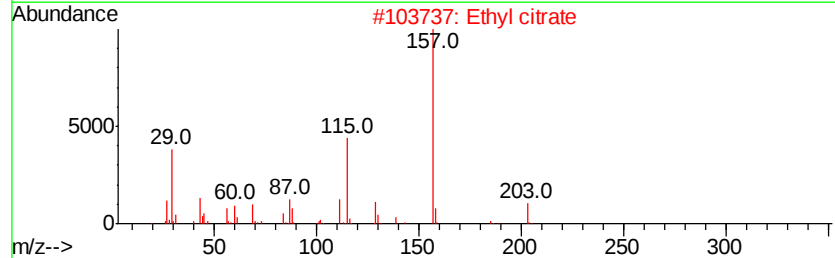
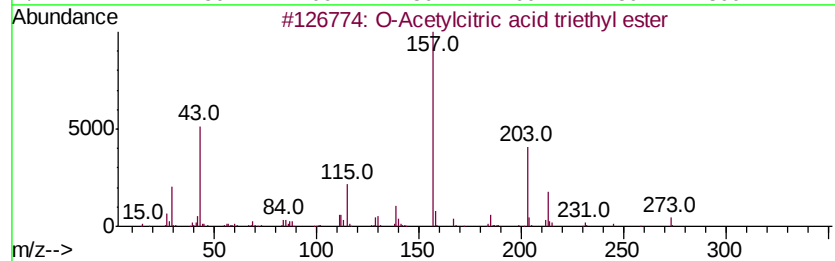
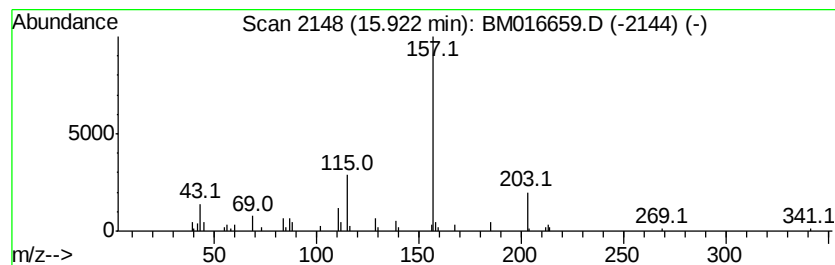
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Peak Number 3 O-Acetylcitric acid triethy... Concentration Rank 3

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 15.92 | 2.45 ng | 88022 | Acenaphthene-d10 | 14.63 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#         | Qual |
|------|----|-------------------------------------|-----|------------|--------------|------|
| 1    | 5  | O-Acetylcitric acid triethyl ester  | 318 | C14H22O8   | 000077-89-4  | 64   |
| 2    |    | Ethyl citrate                       | 276 | C12H20O7   | 000077-93-0  | 56   |
| 3    |    | Octanedioic acid, bis(1-methylpr... | 286 | C16H30O4   | 057983-35-4  | 33   |
| 4    |    | 1-Methyl-1-(6-ethyloct-3-yl)oxy-... | 256 | C15H32O5   | 1000216-91-3 | 28   |
| 5    |    | 2-Chlorobenzoic acid, pentadecyl... | 366 | C22H35ClO2 | 1000292-43-0 | 28   |



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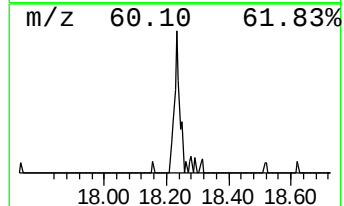
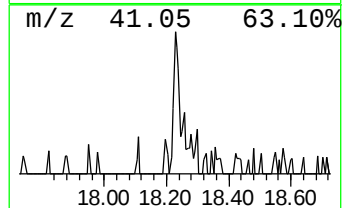
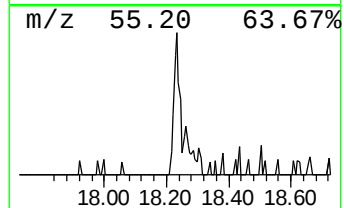
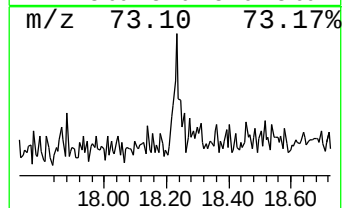
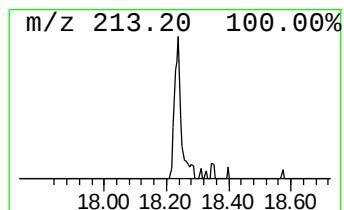
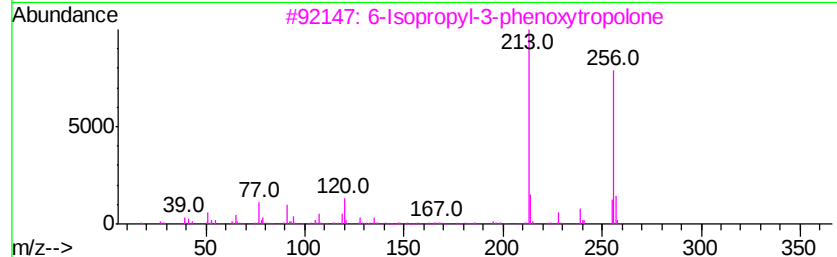
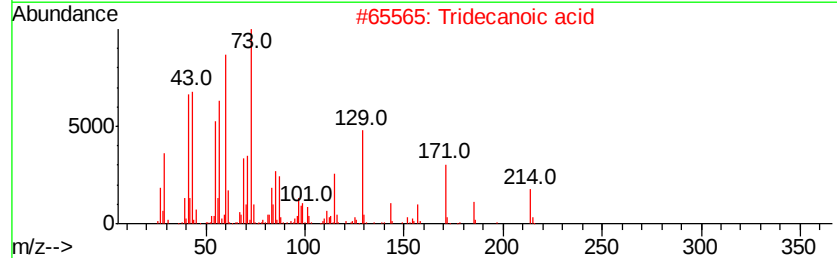
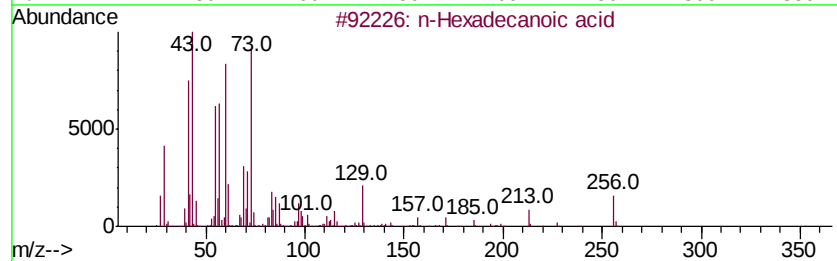
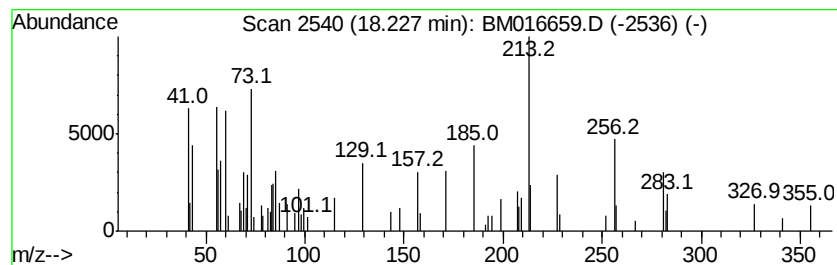
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ClientSampleId :  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

| R.T.    | EstConc | Area                           | Relative to ISTD |          | R.T.        |      |
|---------|---------|--------------------------------|------------------|----------|-------------|------|
| 18.23   | 2.27 ng | 107651                         | Phenanthrene-d10 |          | 17.38       |      |
| Hit# of | 5       | Tentative ID                   | MW               | MolForm  | CAS#        | Qual |
| 1       |         | n-Hexadecanoic acid            | 256              | C16H32O2 | 000057-10-3 | 55   |
| 2       |         | Tridecanoic acid               | 214              | C13H26O2 | 000638-53-9 | 38   |
| 3       |         | 6-Isopropyl-3-phenoxytropolone | 256              | C16H16O3 | 002904-79-2 | 22   |
| 4       |         | n-Decanoic acid                | 172              | C10H20O2 | 000334-48-5 | 22   |
| 5       |         | Tetradecanoic acid             | 228              | C14H28O2 | 000544-63-8 | 20   |



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BNA\_M  
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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown7.52          | 7.52  | 58.1    | ng    | 1426750  | 1                     | 7.99  | 490791 | 20.0 |
| 0-Acetylcitric ac... | 15.92 | 2.5     | ng    | 88022    | 3                     | 14.63 | 719380 | 20.0 |
| n-Hexadecanoic acid  | 18.23 | 2.3     | ng    | 107651   | 4                     | 17.38 | 946817 | 20.0 |