

Data Path : Z:\HPCHEM1\BNA M\DATA\BM052617\  
 Data File : BM010252.D  
 Acq On : 26 May 2017 12:11  
 Operator : SJ/MA  
 Sample : I3332-08  
 Misc :  
 ALS Vial : 5 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 SB-15COMP

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

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         | 5.063       | 332           | 336         | 343          | rBV      | 129521         | 185190        | 3.12%           | 0.538%        |
| 2         | 5.522       | 408           | 414         | 424          | rBV      | 1832954        | 2613065       | 43.99%          | 7.594%        |
| 3         | 7.128       | 678           | 687         | 701          | rBV      | 1642852        | 2594376       | 43.68%          | 7.539%        |
| 4         | 7.481       | 740           | 747         | 757          | rBV      | 1779254        | 2754713       | 46.37%          | 8.005%        |
| 5         | 7.940       | 816           | 825         | 832          | rBV      | 481039         | 763845        | 12.86%          | 2.220%        |
| 6         | 8.263       | 872           | 880         | 890          | rBV      | 1255559        | 2003903       | 33.73%          | 5.823%        |
| 7         | 9.128       | 1019          | 1027        | 1035         | rBV      | 943722         | 1540135       | 25.93%          | 4.476%        |
| 8         | 10.745      | 1294          | 1302        | 1309         | rBV      | 554729         | 905846        | 15.25%          | 2.632%        |
| 9         | 13.192      | 1712          | 1718        | 1731         | rVB      | 2248622        | 3104712       | 52.27%          | 9.023%        |
| 10        | 14.033      | 1854          | 1861        | 1873         | rBV      | 657415         | 914286        | 15.39%          | 2.657%        |
| 11        | 14.575      | 1945          | 1953        | 1962         | rBV2     | 794441         | 1213383       | 20.43%          | 3.526%        |
| 12        | 16.063      | 2200          | 2206        | 2215         | rBV      | 2190389        | 3012565       | 50.72%          | 8.755%        |
| 13        | 16.216      | 2227          | 2232        | 2242         | rVB2     | 38265          | 66395         | 1.12%           | 0.193%        |
| 14        | 17.316      | 2412          | 2419        | 2426         | rBV2     | 1075111        | 1568470       | 26.40%          | 4.558%        |
| 15        | 18.169      | 2559          | 2564        | 2569         | rBV      | 106048         | 183212        | 3.08%           | 0.532%        |
| 16        | 19.439      | 2776          | 2780        | 2783         | rBV4     | 41332          | 62035         | 1.04%           | 0.180%        |
| 17        | 19.921      | 2856          | 2862        | 2869         | rBV      | 4977611        | 5940177       | 100.00%         | 17.263%       |
| 18        | 21.480      | 3122          | 3127        | 3134         | rBV      | 1890395        | 2391448       | 40.26%          | 6.950%        |
| 19        | 23.839      | 3522          | 3528        | 3537         | rVB2     | 1276689        | 2592997       | 43.65%          | 7.535%        |

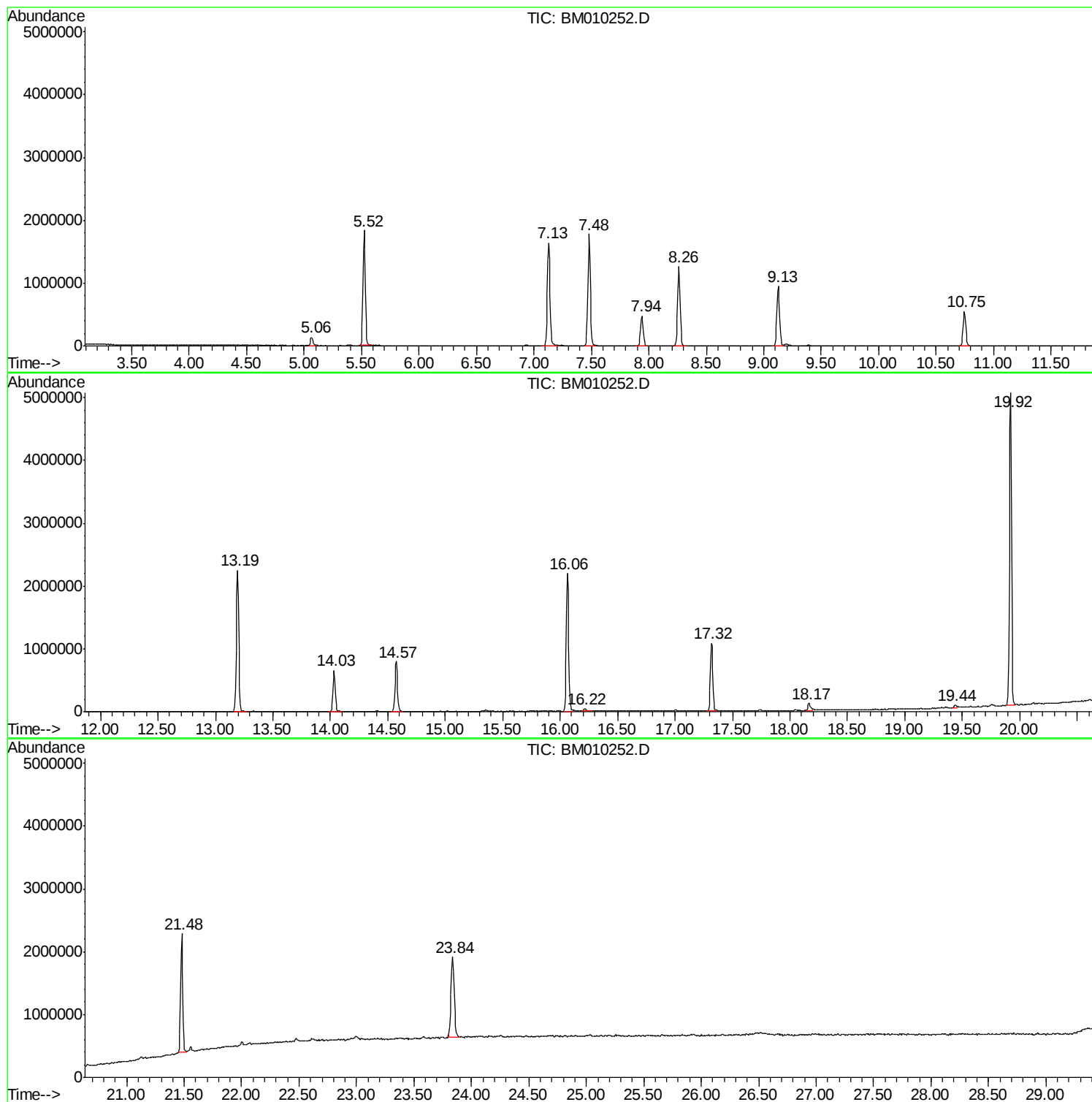
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Quant Method : Z:\HPCHEM1\BNA M\METHODS\8270-BM051917.M  
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TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



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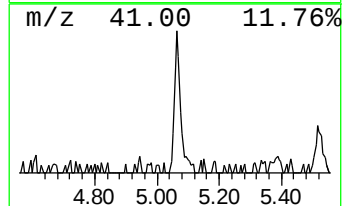
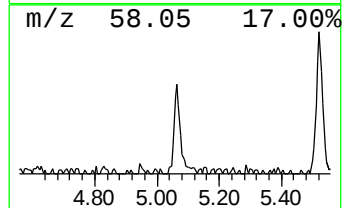
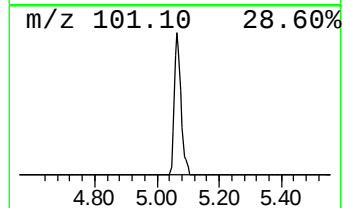
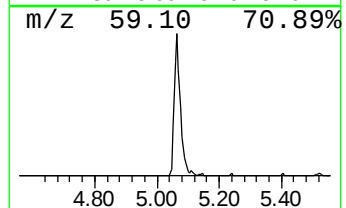
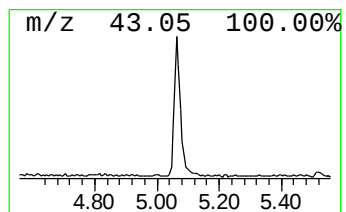
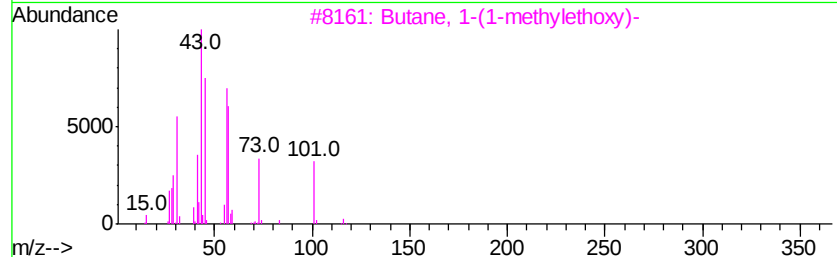
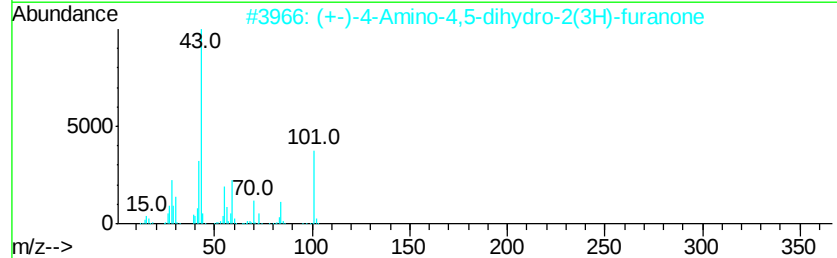
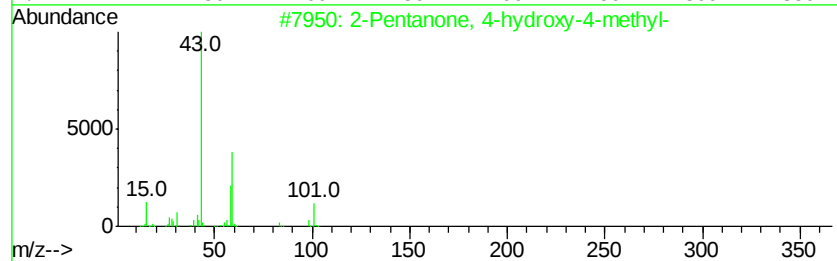
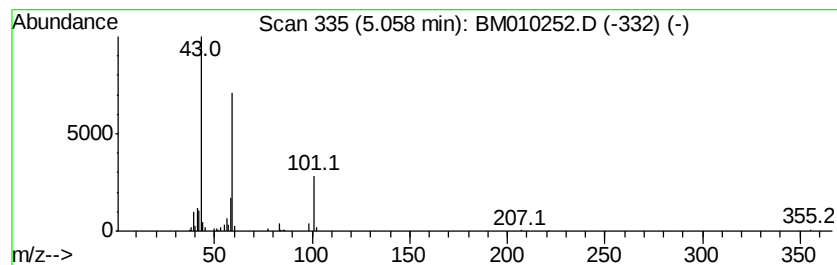
TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

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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. |
|------|---------|--------|------------------------|------|
| 5.06 | 4.85 ng | 185190 | 1,4-Dichlorobenzene-d4 | 7.94 |

| Hit# | of | 5 | Tentative ID                           | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------------------------|-----|---------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-       | 116 | C6H12O2 | 000123-42-2 | 50   |
| 2    |    |   | (+)-4-Amino-4,5-dihydro-2(3H)-furanone | 101 | C4H7NO2 | 016504-58-8 | 38   |
| 3    |    |   | Butane, 1-(1-methylethoxy)-            | 116 | C7H16O  | 001860-27-1 | 32   |
| 4    |    |   | tert-Butyl Hydroperoxide               | 90  | C4H10O2 | 000075-91-2 | 28   |
| 5    |    |   | Butyl aldoxime, 3-methyl-, syn-        | 101 | C5H11NO | 005780-40-5 | 25   |



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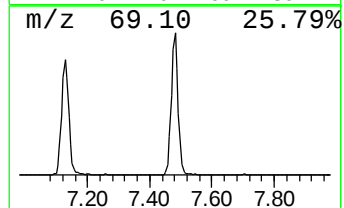
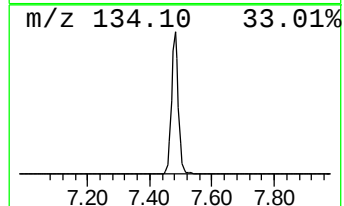
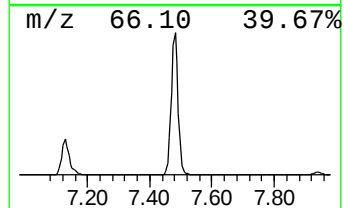
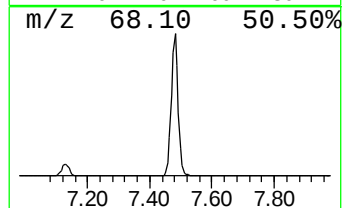
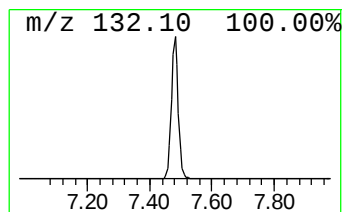
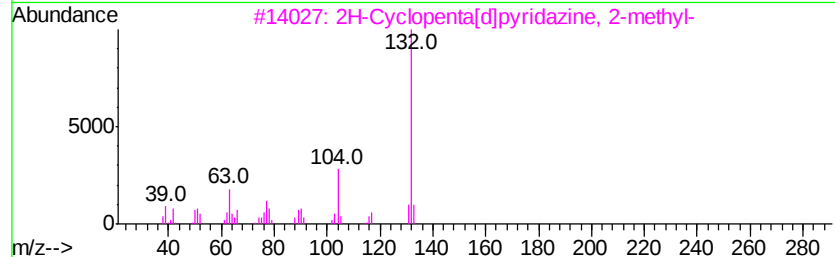
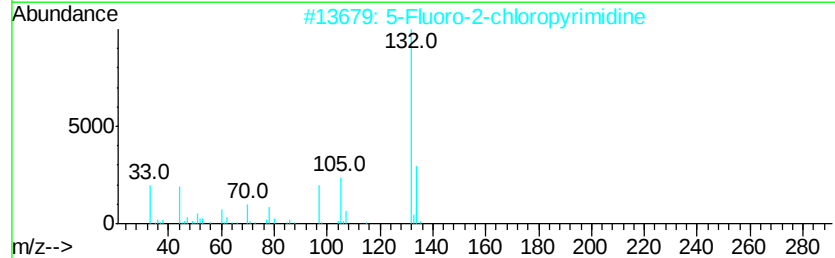
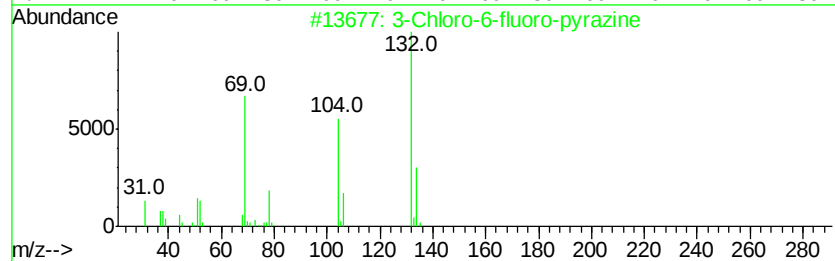
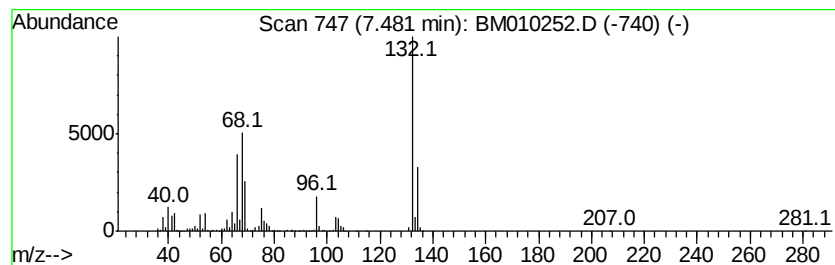
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Peak Number 2 unknown7.48 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 7.48 | 72.13 ng | 2754710 | 1,4-Dichlorobenzene-d4 | 7.94 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 14   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 14   |
| 3    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 14   |
| 4    |    | 1,3-Cyclopentanedione, 2-chloro-    | 132 | C5H5ClO2  | 014203-19-1  | 12   |
| 5    |    | Benzene, 1,2,4-trifluoro-           | 132 | C6H3F3    | 000367-23-7  | 10   |



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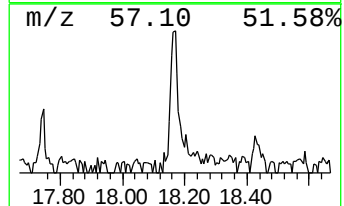
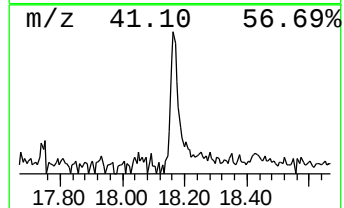
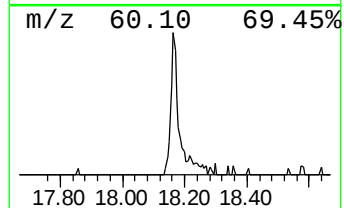
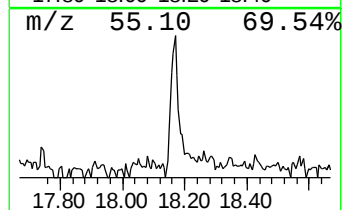
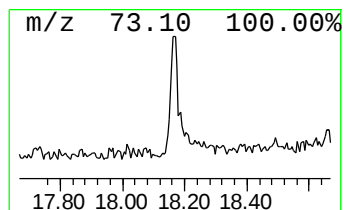
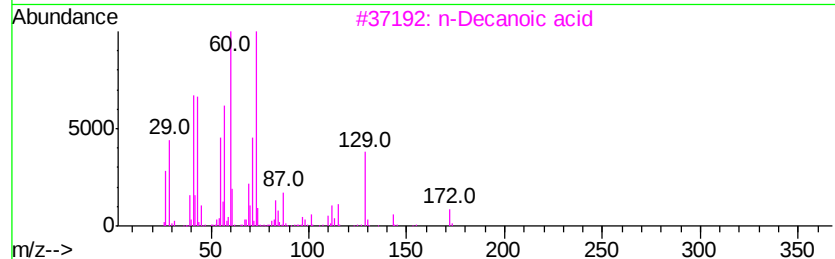
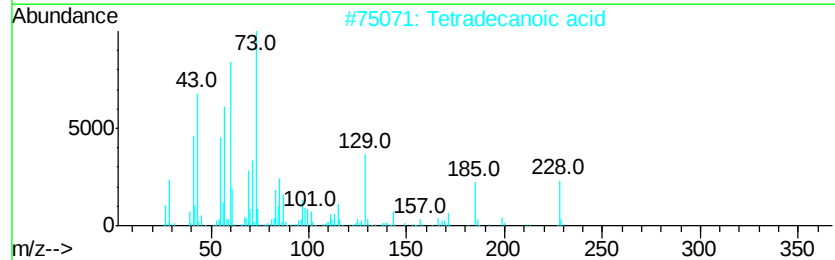
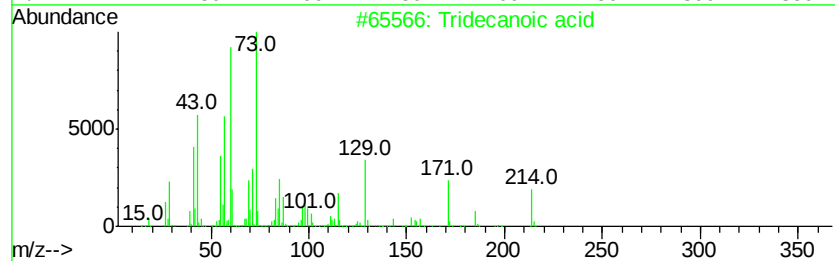
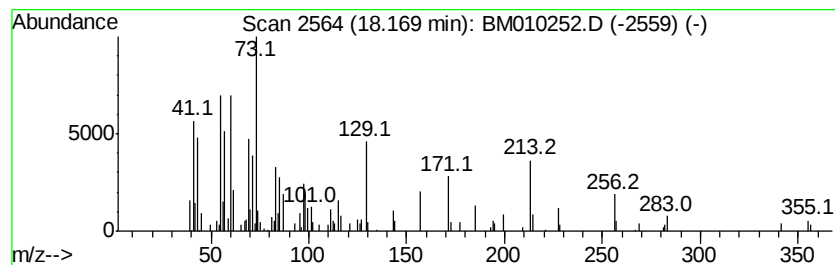
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TIC Integration Parameters: LSCINT.P

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Peak Number 4 Tridecanoic acid Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 18.17 | 2.34 ng | 183212 | Phenanthrene-d10 | 17.32 |

| Hit# of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|---------|---|-------------------------------------|-----|-----------|-------------|------|
| 1       |   | Tridecanoic acid                    | 214 | C13H26O2  | 000638-53-9 | 93   |
| 2       |   | Tetradecanoic acid                  | 228 | C14H28O2  | 000544-63-8 | 70   |
| 3       |   | n-Decanoic acid                     | 172 | C10H20O2  | 000334-48-5 | 53   |
| 4       |   | Dodecanoic acid                     | 200 | C12H24O2  | 000143-07-7 | 47   |
| 5       |   | D-Glucose, 4-O-.alpha.-D-glucopy... | 342 | C12H22O11 | 000069-79-4 | 35   |



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| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.06  | 4.8     | ng    | 185190   | 1                     | 7.94  | 763845  | 20.0 |
| unknown7.48          | 7.48  | 72.1    | ng    | 2754710  | 1                     | 7.94  | 763845  | 20.0 |
| Tridecanoic acid     | 18.17 | 2.3     | ng    | 183212   | 4                     | 17.32 | 1568470 | 20.0 |