

Data Path : Z:\svoasrv\HPCHEM1\BNA\_M\Data\BM080323\  
 Data File : BM041255.D  
 Acq On : 03 Aug 2023 10:11  
 Operator : MA/JU  
 Sample : PB154308BL  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_M  
 ClientSampleId :  
 PB154308BL

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:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM041255.D\data.ms

| 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         | 5.369       | 365           | 371         | 382          | rBV      | 279401         | 424299        | 21.97%          | 2.930%        |
| 2         | 6.975       | 638           | 644         | 656          | rBV      | 262181         | 433198        | 22.43%          | 2.991%        |
| 3         | 7.792       | 776           | 783         | 792          | rBV      | 485962         | 746738        | 38.66%          | 5.157%        |
| 4         | 8.969       | 976           | 983         | 993          | rBV      | 160613         | 276553        | 14.32%          | 1.910%        |
| 5         | 10.598      | 1252          | 1260        | 1269         | rBV      | 631523         | 1048714       | 54.30%          | 7.242%        |
| 6         | 12.192      | 1519          | 1531        | 1540         | rBV      | 6765           | 25193         | 1.30%           | 0.174%        |
| 7         | 13.074      | 1675          | 1681        | 1691         | rVB      | 455990         | 670909        | 34.74%          | 4.633%        |
| 8         | 14.339      | 1882          | 1896        | 1909         | rBV      | 190441         | 583887        | 30.23%          | 4.032%        |
| 9         | 14.463      | 1911          | 1917        | 1933         | rVB      | 982752         | 1465549       | 75.88%          | 10.120%       |
| 10        | 14.886      | 1982          | 1989        | 2000         | rBV2     | 32465          | 73822         | 3.82%           | 0.510%        |
| 11        | 15.257      | 2047          | 2052        | 2056         | rBV4     | 9568           | 19790         | 1.02%           | 0.137%        |
| 12        | 15.962      | 2166          | 2172        | 2182         | rBV      | 358333         | 530863        | 27.49%          | 3.666%        |
| 13        | 17.221      | 2380          | 2386        | 2397         | rBV      | 1259456        | 1754024       | 90.82%          | 12.112%       |
| 14        | 18.121      | 2534          | 2539        | 2550         | rBV      | 511126         | 888193        | 45.99%          | 6.133%        |
| 15        | 18.668      | 2628          | 2632        | 2638         | rBV7     | 16236          | 24894         | 1.29%           | 0.172%        |
| 16        | 19.262      | 2730          | 2733        | 2735         | rBV3     | 15194          | 21892         | 1.13%           | 0.151%        |
| 17        | 19.403      | 2752          | 2757        | 2772         | rBV      | 284577         | 549861        | 28.47%          | 3.797%        |
| 18        | 19.856      | 2829          | 2834        | 2843         | rBV      | 881397         | 1094478       | 56.67%          | 7.558%        |
| 19        | 21.427      | 3096          | 3101        | 3108         | rBV      | 1525779        | 1916996       | 99.26%          | 13.238%       |
| 20        | 23.797      | 3498          | 3504        | 3516         | rVB      | 979095         | 1931329       | 100.00%         | 13.337%       |

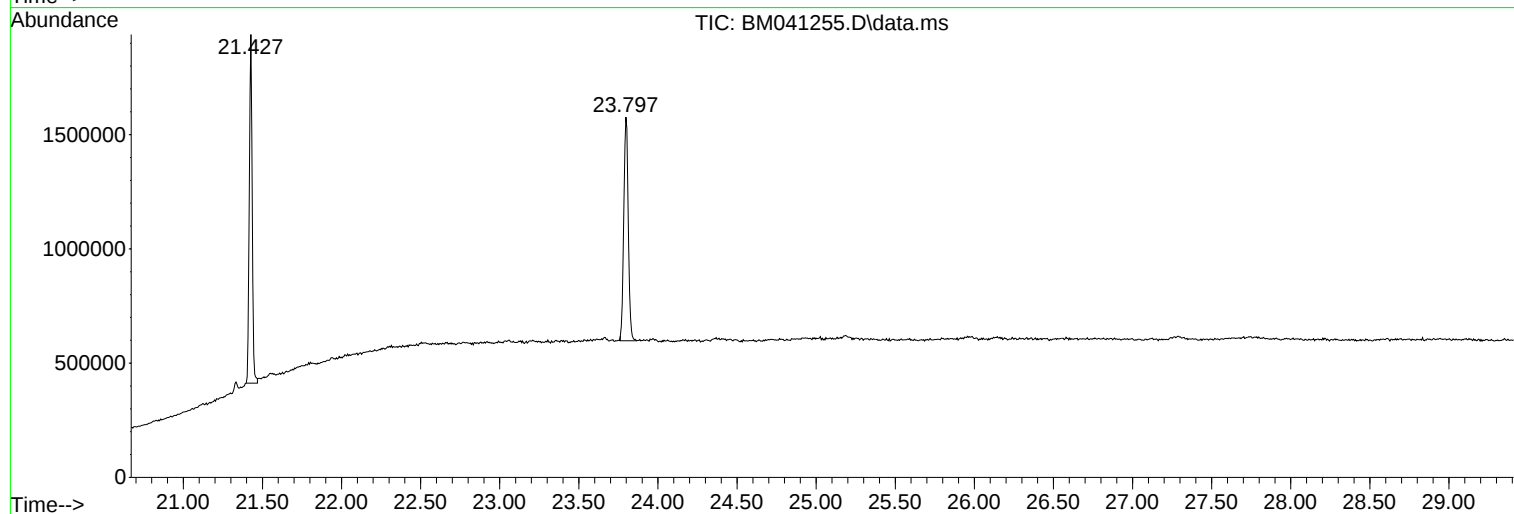
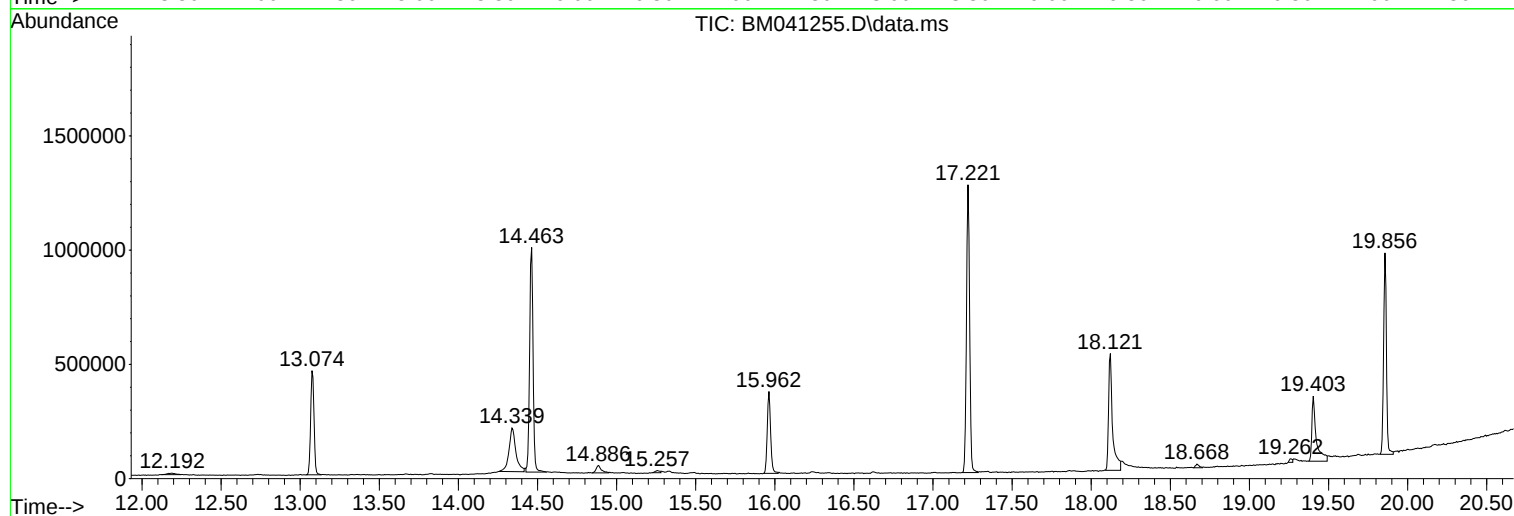
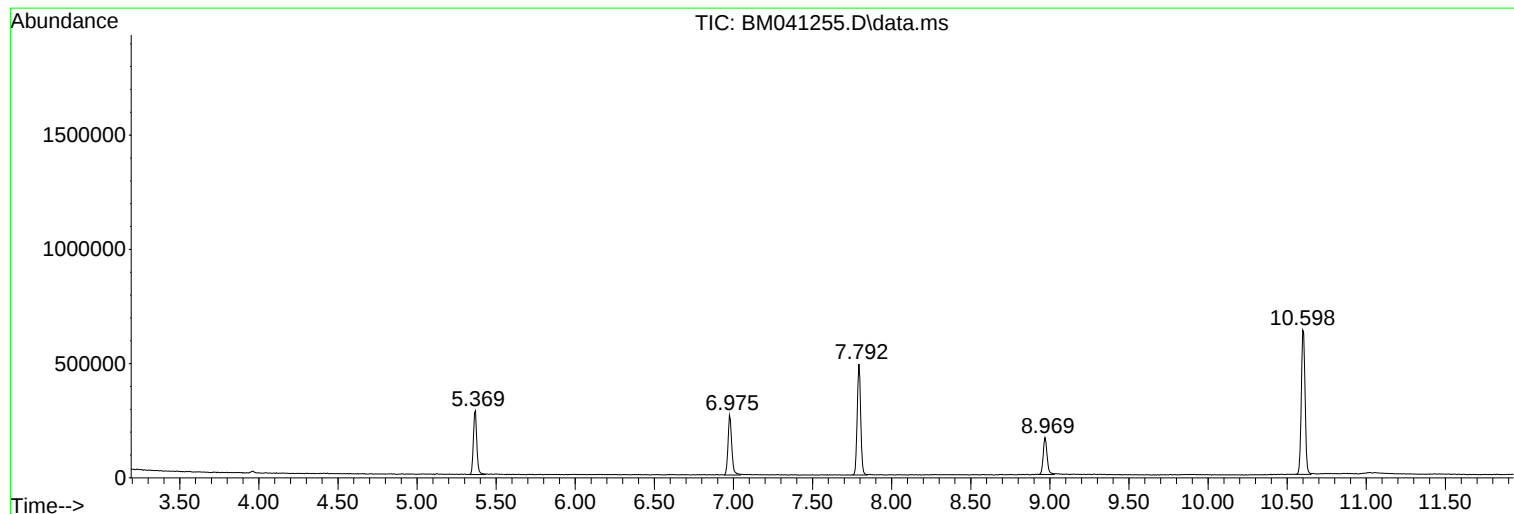
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ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_M  
ClientSampleId :  
PB154308BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P



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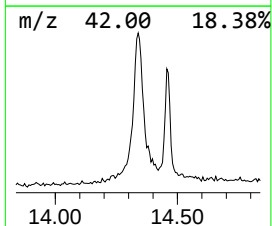
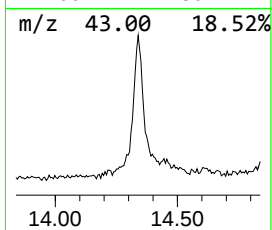
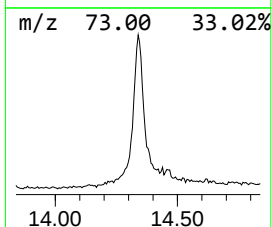
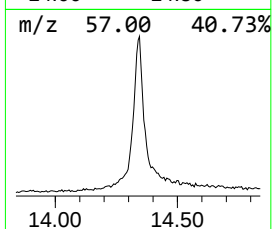
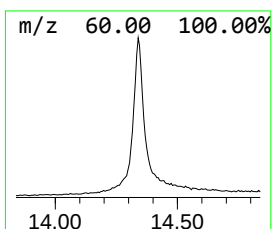
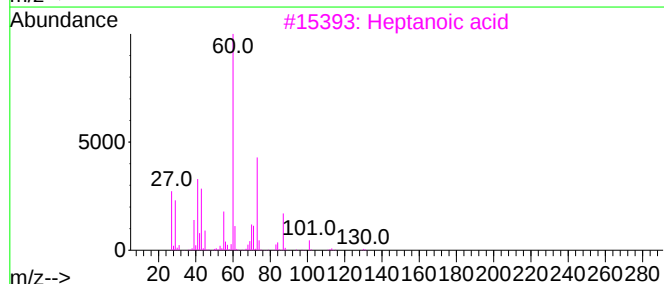
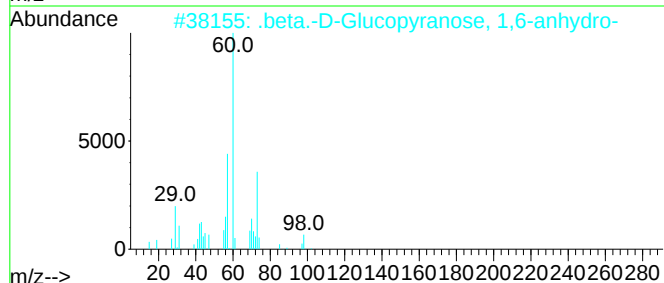
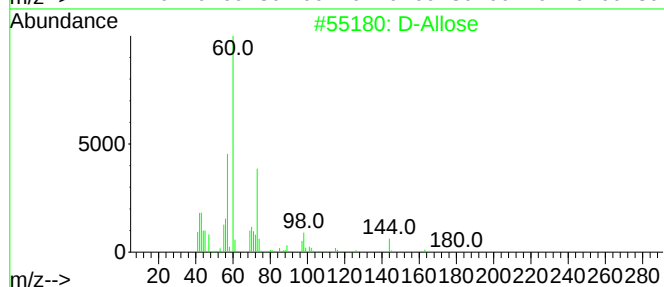
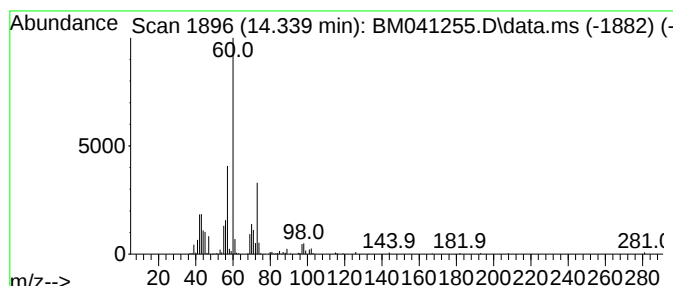
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 D-Allose Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.339 | 7.97 ng | 583887 | Acenaphthene-d10 | 14.463 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | D-Allose                            | 180 | C6H12O6 | 002595-97-3 | 90   |
| 2    |    |   | .beta.-D-Glucopyranose, 1,6-anhy... | 162 | C6H10O5 | 000498-07-7 | 72   |
| 3    |    |   | Heptanoic acid                      | 130 | C7H14O2 | 000111-14-8 | 64   |
| 4    |    |   | Ethyl .alpha.-d-glucopyranoside     | 208 | C8H16O6 | 019467-01-7 | 53   |
| 5    |    |   | Butanoic acid                       | 88  | C4H8O2  | 000107-92-6 | 53   |



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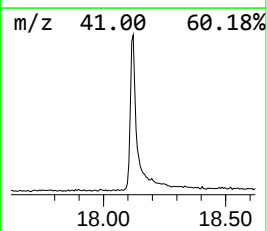
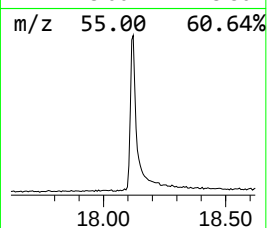
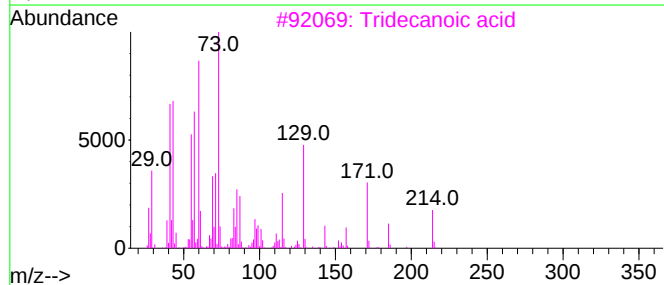
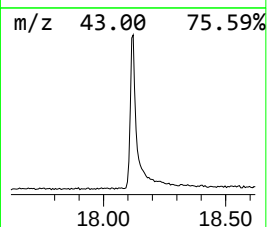
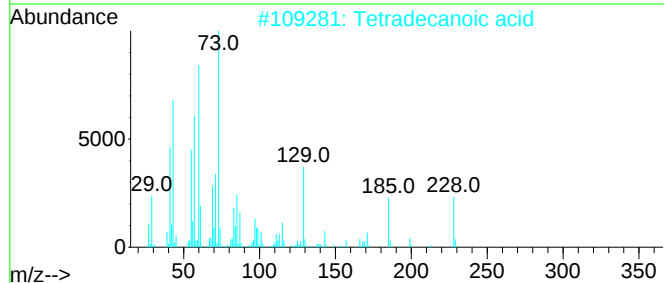
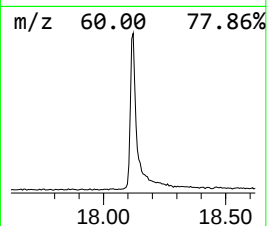
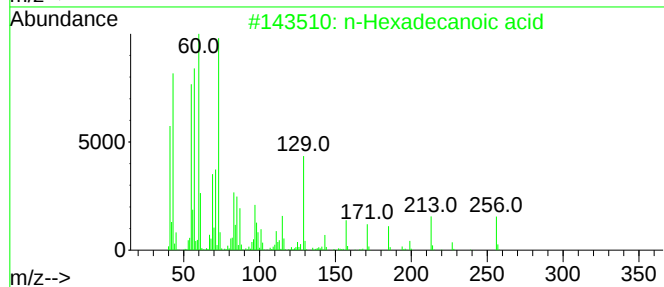
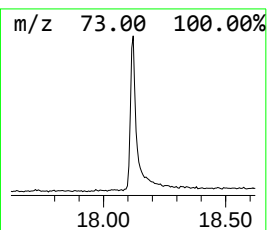
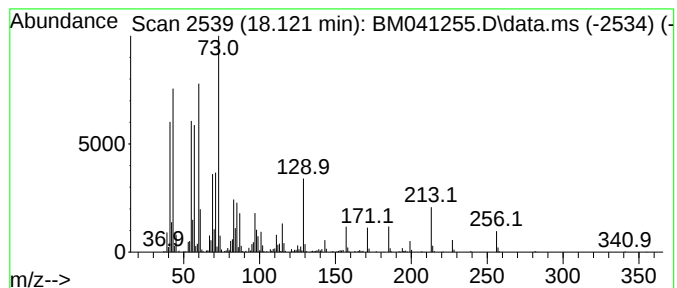
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L  
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc  | Area   | Relative to ISTD | R.T.   |
|--------|----------|--------|------------------|--------|
| 18.121 | 10.13 ng | 888193 | Phenanthrene-d10 | 17.221 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 94   |
| 3    |    |   | Tridecanoic acid    | 214 | C13H26O2 | 000638-53-9 | 93   |
| 4    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 81   |
| 5    |    |   | Octadecanoic acid   | 284 | C18H36O2 | 000057-11-4 | 76   |



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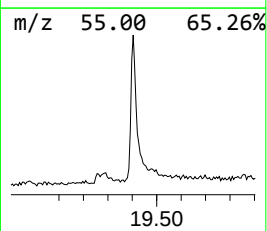
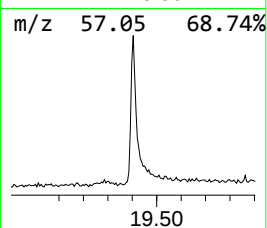
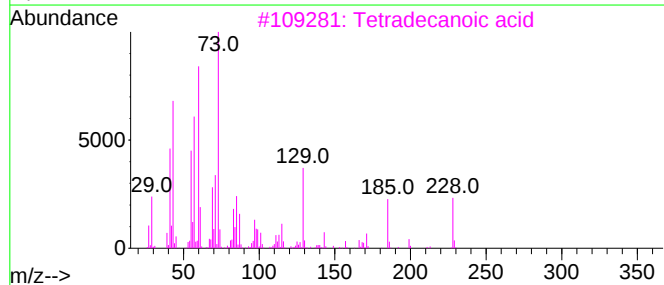
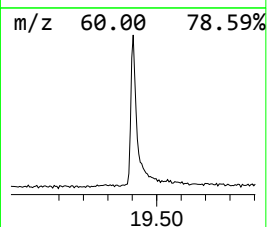
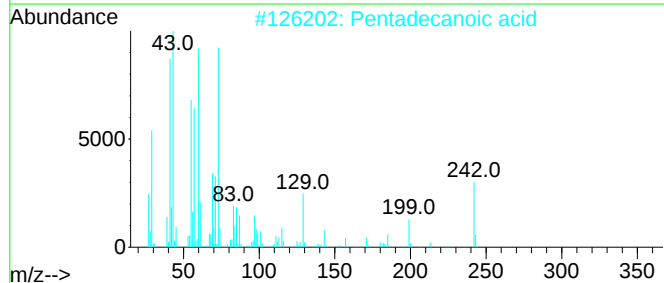
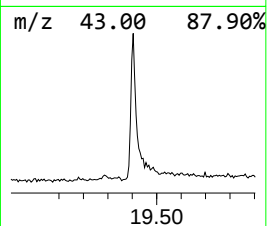
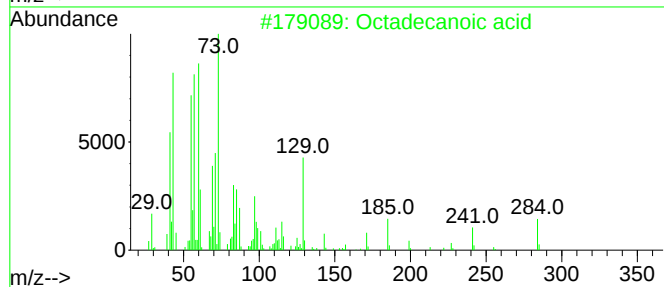
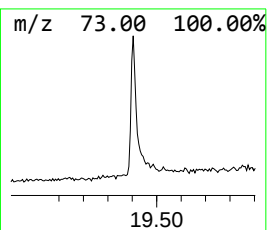
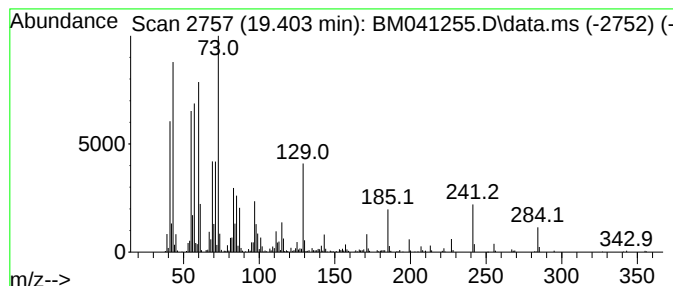
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TIC Library : C:\Database\NIST20.L  
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Peak Number 3 Octadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 19.403 | 5.74 ng | 549861 | Chrysene-d12     | 21.427 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Octadecanoic acid                   | 284 | C18H36O2 | 000057-11-4 | 99   |
| 2    |    |   | Pentadecanoic acid                  | 242 | C15H30O2 | 001002-84-2 | 91   |
| 3    |    |   | Tetradecanoic acid                  | 228 | C14H28O2 | 000544-63-8 | 87   |
| 4    |    |   | Octadecanoic acid, 2-(2-hydroxye... | 372 | C22H44O4 | 000106-11-6 | 83   |
| 5    |    |   | Tridecanoic acid                    | 214 | C13H26O2 | 000638-53-9 | 76   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_M\Methods\8270-BM072823.M  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| D-Allose           | 14.339 | 8.0     | ng    | 583887   | 3                     | 14.463 | 1465550 | 20.0 |
| n-Hexadecanoic ... | 18.121 | 10.1    | ng    | 888193   | 4                     | 17.221 | 1754020 | 20.0 |
| Octadecanoic acid  | 19.403 | 5.7     | ng    | 549861   | 5                     | 21.427 | 1917000 | 20.0 |