

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF112823\  
 Data File : BF136268.D  
 Acq On : 29 Nov 2023 01:21  
 Operator : CG\JU  
 Sample : 05547-03  
 Misc :  
 ALS Vial : 19 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 BCC-8002

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\_F\Methods\8270-BF112723.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136268.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         | 5.040       | 499           | 502         | 509          | rVB      | 33836          | 38804         | 1.61%           | 0.247%        |
| 2         | 5.440       | 565           | 570         | 573          | rBV      | 2699800        | 2275063       | 94.55%          | 14.472%       |
| 3         | 6.434       | 734           | 739         | 742          | rBV      | 2174468        | 2149985       | 89.35%          | 13.677%       |
| 4         | 6.804       | 798           | 802         | 805          | rBV      | 866083         | 634190        | 26.36%          | 4.034%        |
| 5         | 7.363       | 892           | 897         | 900          | rBV      | 1640333        | 1325131       | 55.07%          | 8.430%        |
| 6         | 8.081       | 1015          | 1019        | 1022         | rBV      | 1017854        | 755686        | 31.41%          | 4.807%        |
| 7         | 9.157       | 1198          | 1202        | 1205         | rBV      | 3022274        | 2406260       | 100.00%         | 15.307%       |
| 8         | 9.275       | 1220          | 1222        | 1225         | rBV      | 34929          | 31469         | 1.31%           | 0.200%        |
| 9         | 9.839       | 1314          | 1318        | 1321         | rBV      | 747800         | 655195        | 27.23%          | 4.168%        |
| 10        | 10.628      | 1448          | 1452        | 1455         | rBV      | 1249054        | 1056099       | 43.89%          | 6.718%        |
| 11        | 11.328      | 1567          | 1571        | 1576         | rBV      | 750234         | 604588        | 25.13%          | 3.846%        |
| 12        | 11.863      | 1659          | 1662        | 1670         | rBV2     | 97697          | 128435        | 5.34%           | 0.817%        |
| 13        | 12.657      | 1794          | 1797        | 1801         | rBV6     | 33070          | 46658         | 1.94%           | 0.297%        |
| 14        | 12.927      | 1839          | 1843        | 1846         | rBV      | 2844975        | 2330914       | 96.87%          | 14.828%       |
| 15        | 13.980      | 2019          | 2022        | 2029         | rVB      | 723986         | 671376        | 27.90%          | 4.271%        |
| 16        | 14.857      | 2169          | 2171        | 2176         | rVB      | 69257          | 69890         | 2.90%           | 0.445%        |
| 17        | 15.133      | 2215          | 2218        | 2222         | rVB2     | 39500          | 42663         | 1.77%           | 0.271%        |
| 18        | 15.463      | 2270          | 2274        | 2279         | rVB      | 364048         | 430140        | 17.88%          | 2.736%        |
| 19        | 15.733      | 2317          | 2320        | 2325         | rVB2     | 49480          | 67545         | 2.81%           | 0.430%        |

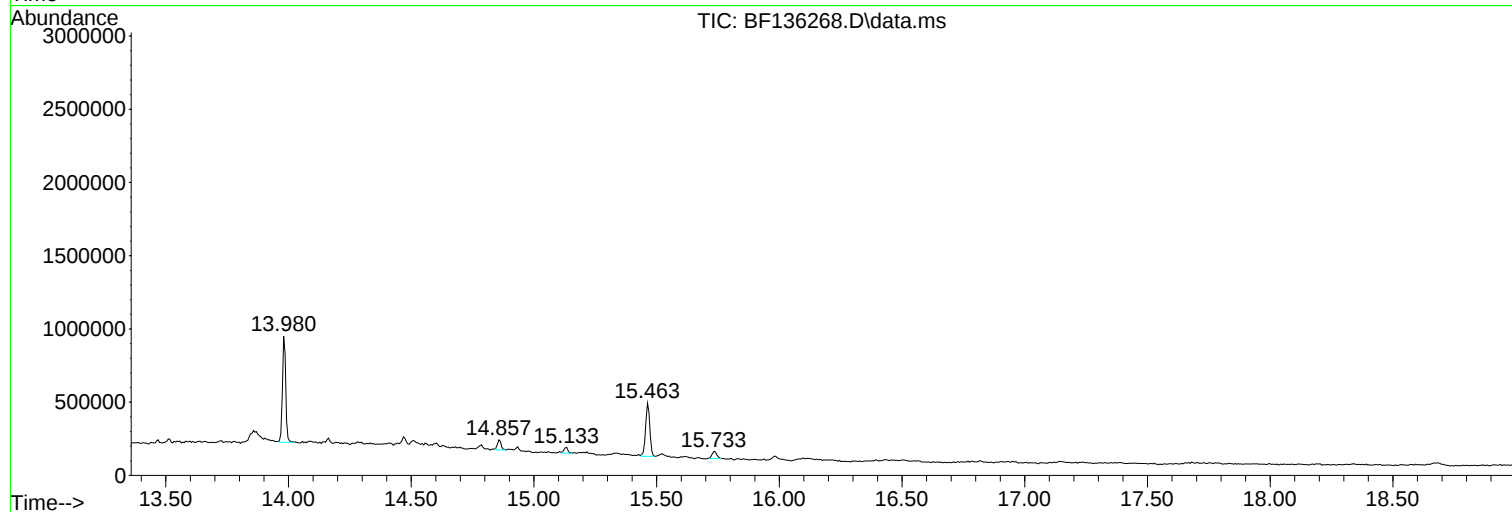
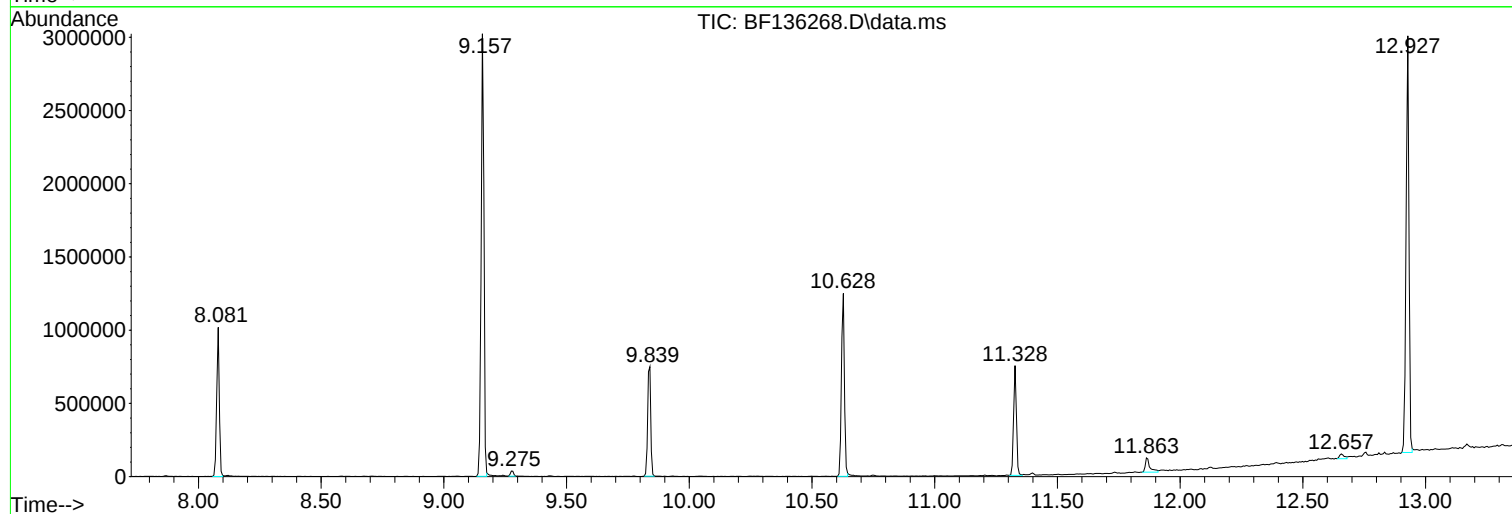
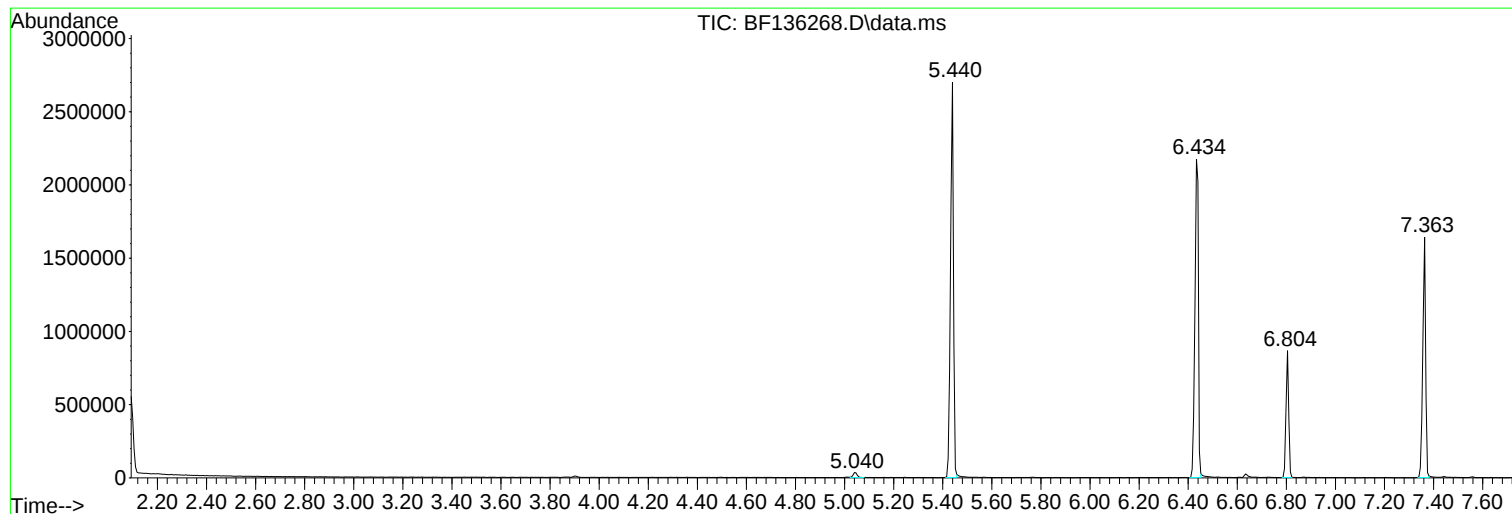
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BNA\_F  
ClientSampleId :  
BCC-8002

Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF112723.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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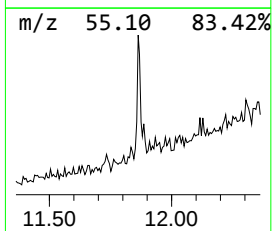
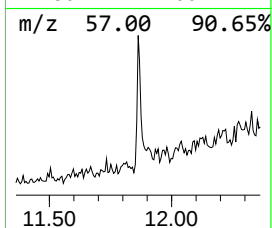
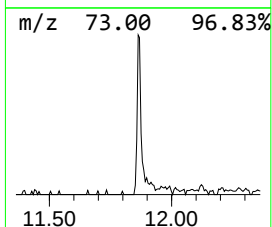
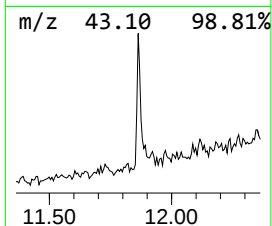
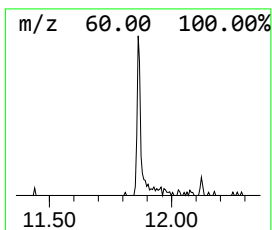
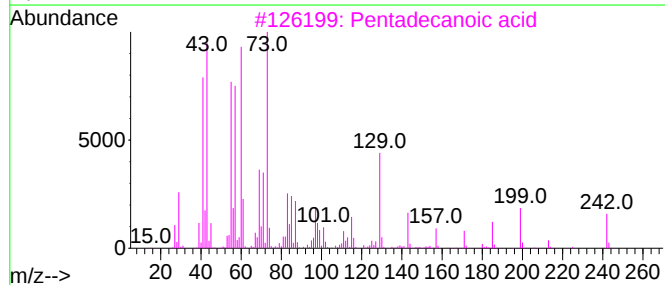
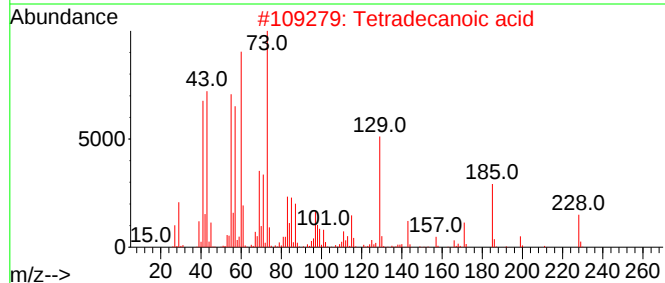
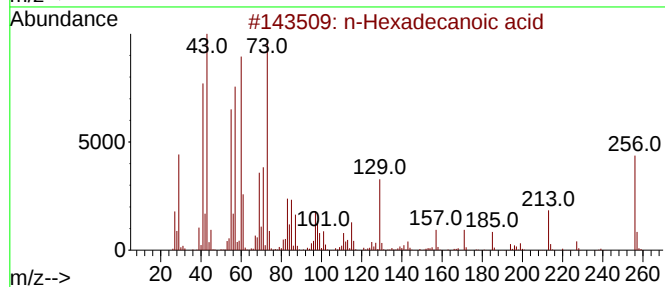
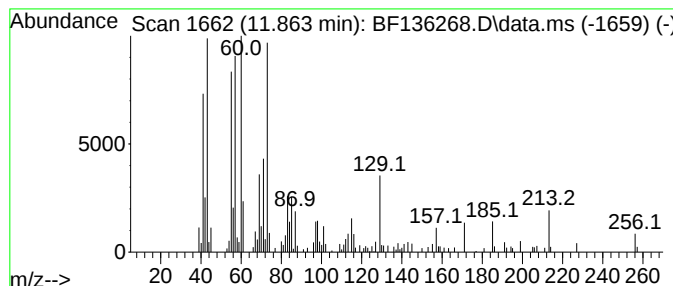
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.863 | 4.25 ng | 128435 | Phenanthrene-d10 | 11.328 |

| Hit# | of | 5 | Tentative ID        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|---------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 96   |
| 2    |    |   | Tetradecanoic acid  | 228 | C14H28O2 | 000544-63-8 | 83   |
| 3    |    |   | Pentadecanoic acid  | 242 | C15H30O2 | 001002-84-2 | 74   |
| 4    |    |   | Dodecanoic acid     | 200 | C12H24O2 | 000143-07-7 | 64   |
| 5    |    |   | Undecanoic acid     | 186 | C11H22O2 | 000112-37-8 | 64   |



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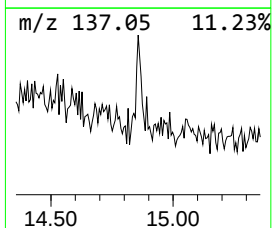
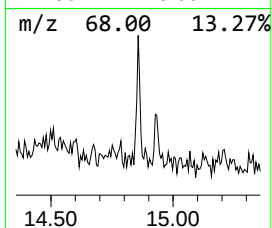
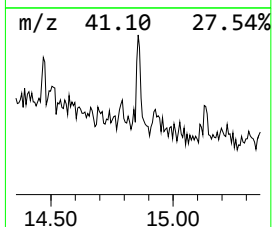
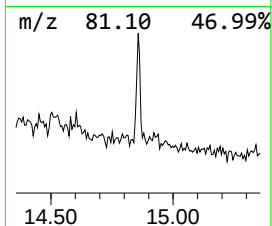
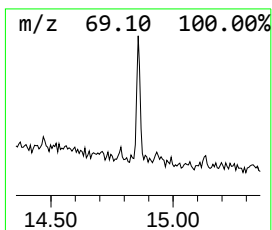
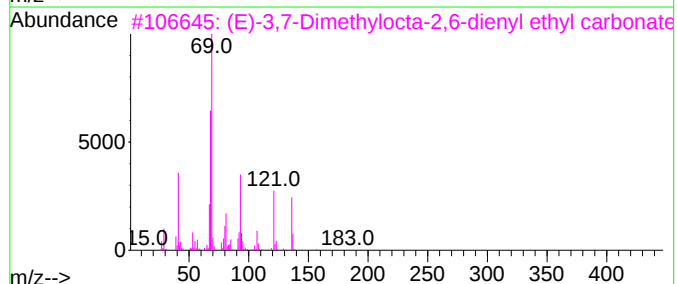
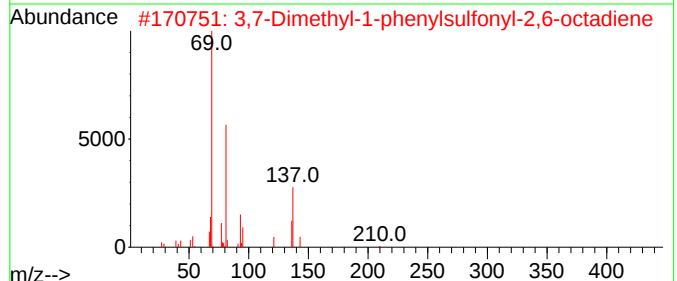
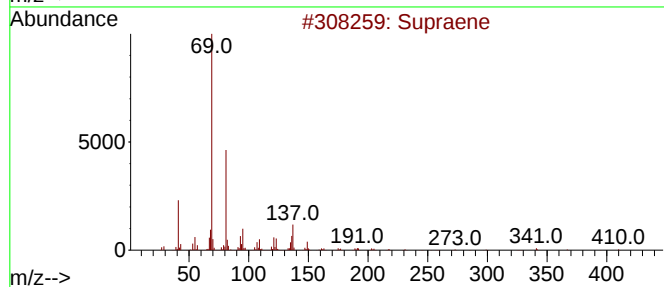
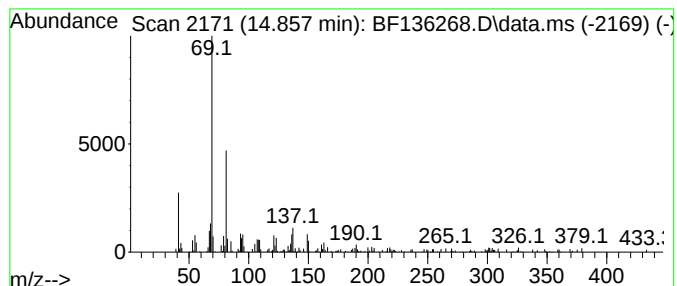
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Peak Number 2 Supraene Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.857 | 3.25 ng | 69890 | Perylene-d12     | 15.463 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50    | 007683-64-9  | 72   |
| 2    |    |   | 3,7-Dimethyl-1-phenylsulfonyl-2,... | 278 | C16H22O2S | 1000432-27-5 | 64   |
| 3    |    |   | (E)-3,7-Dimethylocta-2,6-dienyl ... | 226 | C13H22O3  | 1000373-76-7 | 64   |
| 4    |    |   | 3,7,11-Trimethyl-2,6,10-dodecatr... | 217 | C15H23N   | 029789-67-1  | 64   |
| 5    |    |   | Farnesol isomer a                   | 222 | C15H26O   | 1000108-92-4 | 64   |



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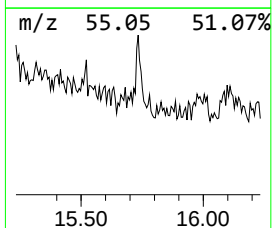
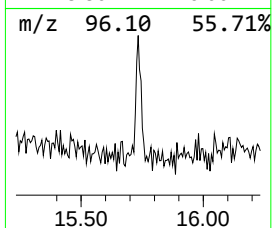
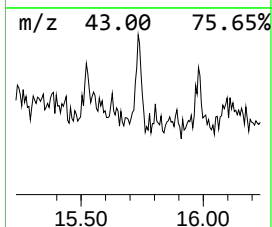
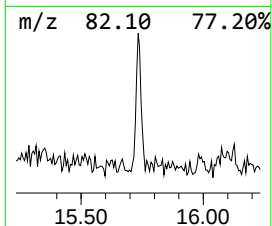
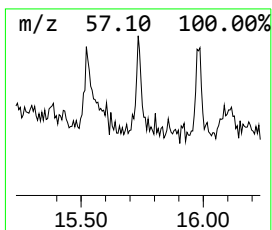
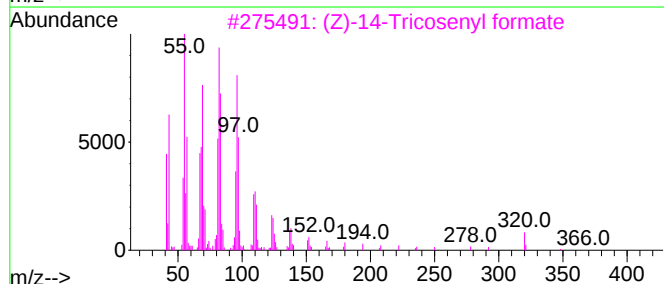
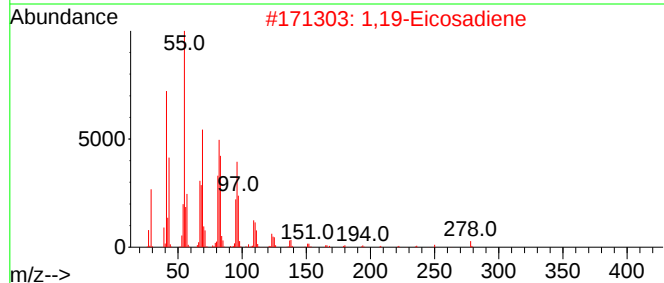
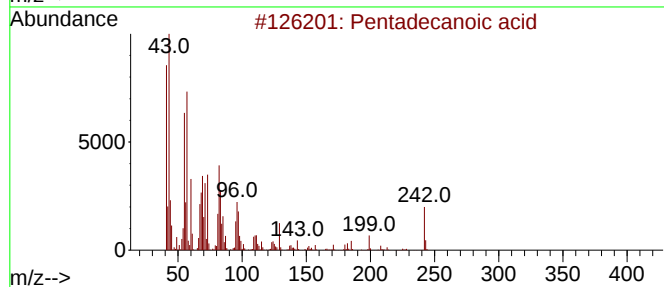
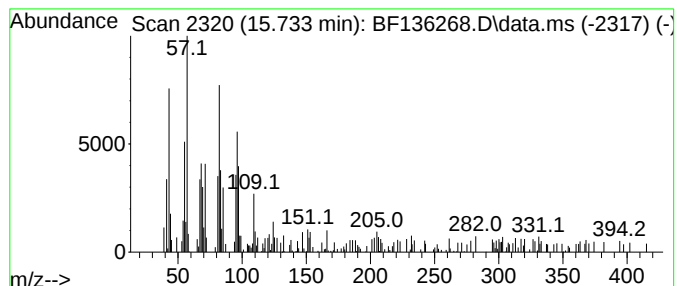
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Pentadecanoic acid Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.733 | 3.14 ng | 67545 | Perylene-d12     | 15.463 |

| Hit# | of | 5 | Tentative ID                  | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------|-----|----------|--------------|------|
| 1    |    |   | Pentadecanoic acid            | 242 | C15H30O2 | 001002-84-2  | 86   |
| 2    |    |   | 1,19-Eicosadiene              | 278 | C20H38   | 014811-95-1  | 81   |
| 3    |    |   | (Z)-14-Tricosenyl formate     | 366 | C24H46O2 | 077899-10-6  | 74   |
| 4    |    |   | Bicyclo[10.8.0]eicosane, cis- | 278 | C20H38   | 1000155-82-2 | 74   |
| 5    |    |   | 1,21-Docosadiene              | 306 | C22H42   | 053057-53-7  | 74   |



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

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| n-Hexadecanoic ... | 11.863 | 4.3     | ng    | 128435   | 4                     | 11.328 | 604588 | 20.0 |
| Supraene           | 14.857 | 3.3     | ng    | 69890    | 6                     | 15.463 | 430140 | 20.0 |
| Pentadecanoic acid | 15.733 | 3.1     | ng    | 67545    | 6                     | 15.463 | 430140 | 20.0 |