

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF030222\  
 Data File : BF127143.D  
 Acq On : 02 Mar 2022 13:16  
 Operator : CG\JU  
 Sample : N1721-05  
 Misc :  
 ALS Vial : 7 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 DUM-3

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-BF021622.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127143.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         | 5.116       | 477           | 481         | 488          | rVB      | 44796          | 54445         | 2.26%           | 0.347%        |
| 2         | 5.516       | 544           | 549         | 552          | rBV      | 2067805        | 1955325       | 81.34%          | 12.450%       |
| 3         | 6.522       | 715           | 720         | 733          | rVB      | 2045747        | 2045655       | 85.10%          | 13.025%       |
| 4         | 6.887       | 779           | 782         | 786          | rBV      | 641968         | 544325        | 22.64%          | 3.466%        |
| 5         | 7.451       | 873           | 878         | 881          | rBV      | 1416624        | 1367077       | 56.87%          | 8.704%        |
| 6         | 8.175       | 996           | 1001        | 1004         | rBV      | 802388         | 717928        | 29.86%          | 4.571%        |
| 7         | 9.251       | 1178          | 1184        | 1187         | rBV      | 2653181        | 2403958       | 100.00%         | 15.306%       |
| 8         | 9.934       | 1296          | 1300        | 1303         | rBV      | 920585         | 786555        | 32.72%          | 5.008%        |
| 9         | 10.722      | 1430          | 1434        | 1437         | rBV      | 1789468        | 1513488       | 62.96%          | 9.636%        |
| 10        | 11.422      | 1549          | 1553        | 1555         | rBV      | 992684         | 780661        | 32.47%          | 4.971%        |
| 11        | 11.445      | 1555          | 1557        | 1560         | rVV      | 78160          | 64520         | 2.68%           | 0.411%        |
| 12        | 11.486      | 1560          | 1564        | 1568         | rVB4     | 22182          | 26017         | 1.08%           | 0.166%        |
| 13        | 12.633      | 1756          | 1759        | 1763         | rBV      | 123895         | 107265        | 4.46%           | 0.683%        |
| 14        | 12.869      | 1793          | 1799        | 1802         | rBV      | 92845          | 97203         | 4.04%           | 0.619%        |
| 15        | 13.010      | 1818          | 1823        | 1826         | rBV      | 2450249        | 2045760       | 85.10%          | 13.025%       |
| 16        | 13.927      | 1970          | 1979        | 1985         | rBV4     | 75225          | 141763        | 5.90%           | 0.903%        |
| 17        | 14.063      | 1998          | 2002        | 2005         | rBV      | 434079         | 403188        | 16.77%          | 2.567%        |
| 18        | 14.910      | 2142          | 2146        | 2150         | rVB      | 100985         | 94380         | 3.93%           | 0.601%        |
| 19        | 15.116      | 2177          | 2181        | 2189         | rBV      | 30709          | 64304         | 2.67%           | 0.409%        |
| 20        | 15.492      | 2242          | 2245        | 2251         | rBV      | 24649          | 27821         | 1.16%           | 0.177%        |
| 21        | 15.557      | 2251          | 2256        | 2266         | rVB2     | 333674         | 427614        | 17.79%          | 2.723%        |
| 22        | 17.063      | 2508          | 2512        | 2520         | rBV2     | 15985          | 36597         | 1.52%           | 0.233%        |

Sum of corrected areas: 15705849



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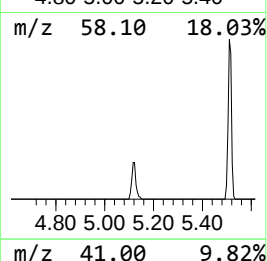
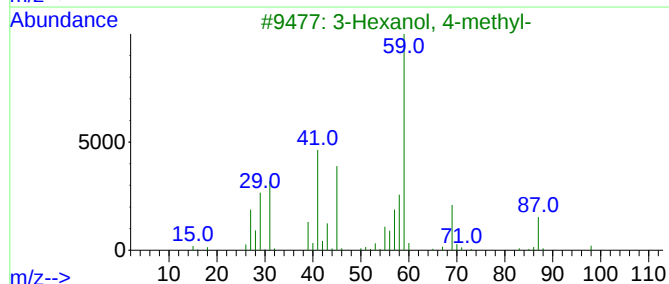
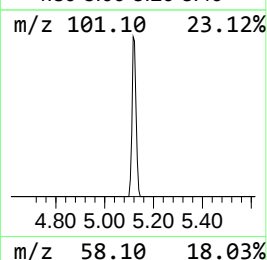
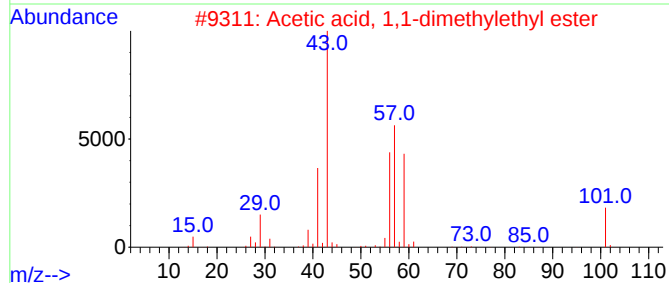
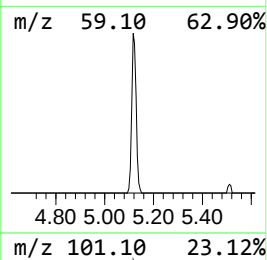
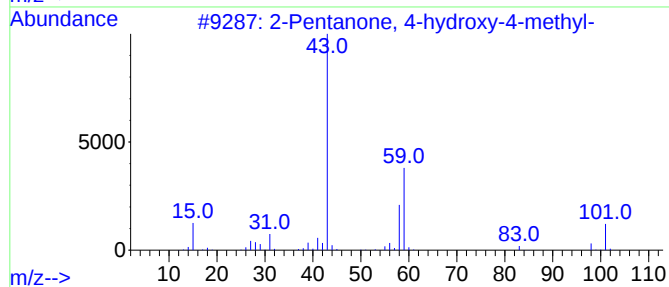
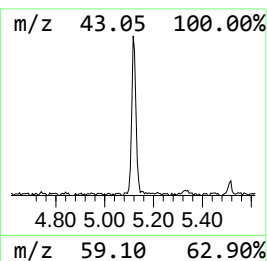
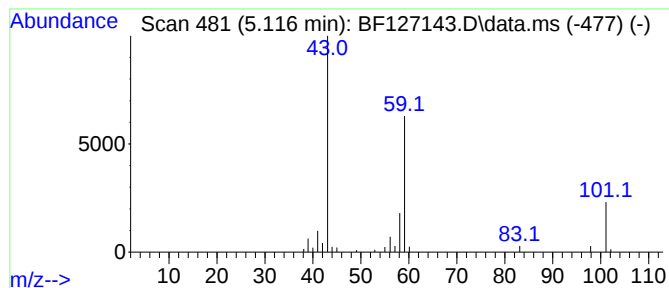
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF021622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

| R.T.  | EstConc | Area  | Relative to ISTD       | R.T.  |
|-------|---------|-------|------------------------|-------|
| 5.116 | 2.00 ng | 54445 | 1,4-Dichlorobenzene-d4 | 6.887 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 72      |      |      |
| 2    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 50      |      |      |
| 3    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 28      |      |      |
| 4    | 1-Butanol, 3-methoxy-               | 104 | C5H12O2      | 002517-43-3 | 25      |      |      |
| 5    | 1,8-Nonanediol, 8-methyl-           | 174 | C10H22O2     | 054725-73-4 | 23      |      |      |



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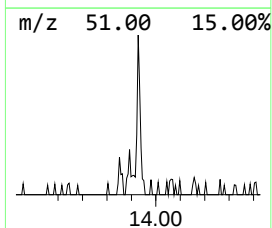
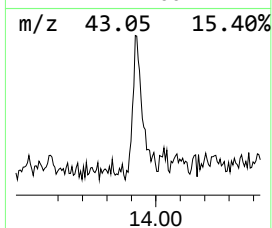
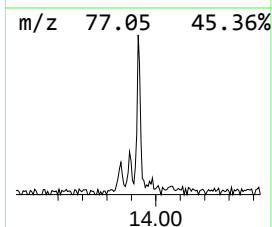
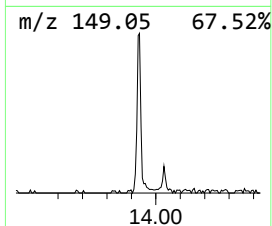
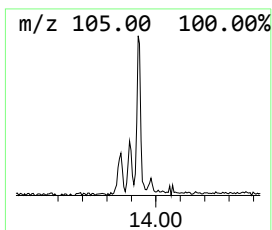
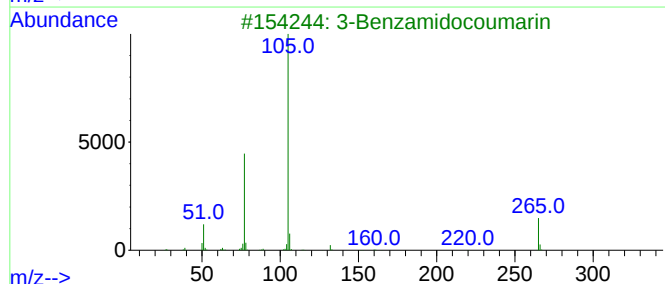
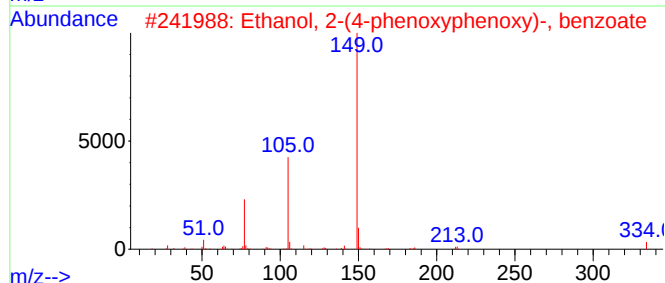
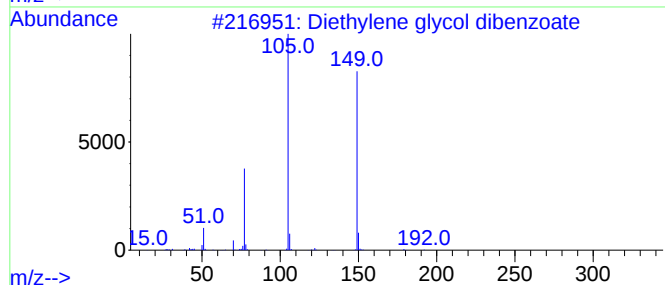
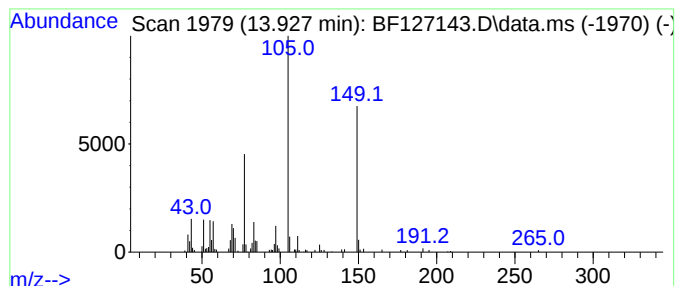
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF021622.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 2 Diethylene glycol dibenzoate Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.928 | 7.03 ng | 141763 | Chrysene-d12     | 14.063 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|-----------|-------------|------|
| 1    |    |   | Diethylene glycol dibenzoate        | 314 | C18H18O5  | 000120-55-8 | 59   |
| 2    |    |   | Ethanol, 2-(4-phenoxyphenoxy)-, ... | 334 | C21H18O4  | 055191-59-8 | 53   |
| 3    |    |   | 3-Benzamidocoumarin                 | 265 | C16H11NO3 | 002549-08-8 | 38   |
| 4    |    |   | Benzoic acid 2-methylpentyl ester   | 206 | C13H18O2  | 059736-57-1 | 38   |
| 5    |    |   | S-Benzoyl(thiohydroxylamine)        | 153 | C7H7NO5   | 025740-80-1 | 35   |



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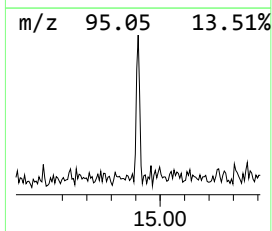
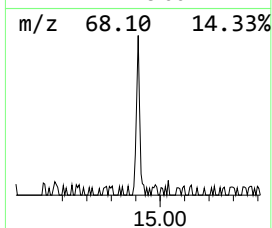
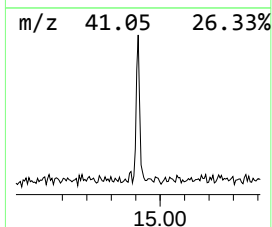
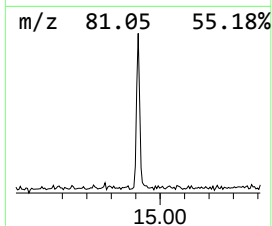
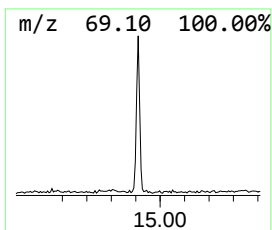
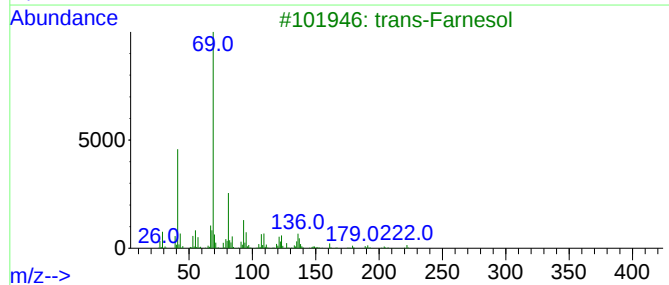
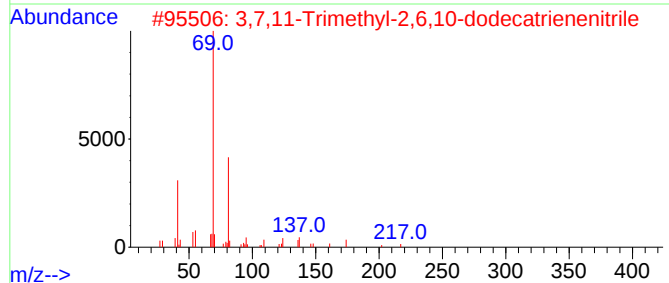
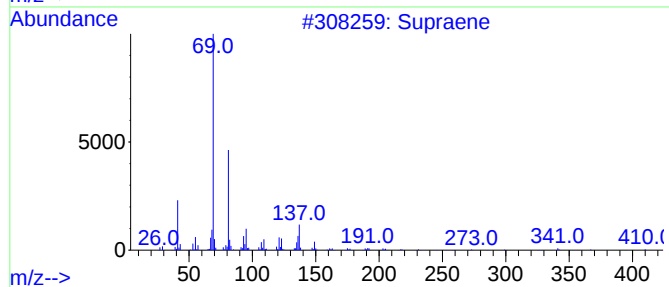
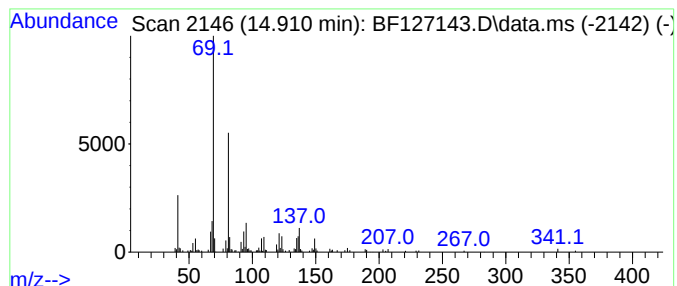
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF021622.M  
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TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Supraene Concentration Rank 2

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.910 | 4.41 ng | 94380 | Perylene-d12     | 15.557 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50  | 007683-64-9 | 91   |
| 2    |    |   | 3,7,11-Trimethyl-2,6,10-dodecatr... | 217 | C15H23N | 029789-67-1 | 64   |
| 3    |    |   | trans-Farnesol                      | 222 | C15H26O | 000106-28-5 | 64   |
| 4    |    |   | 1,5-Heptadiene, 3,3,6-trimethyl-    | 138 | C10H18  | 035387-63-4 | 52   |
| 5    |    |   | 1,5-Heptadiene, 3,4-dimethyl-       | 124 | C9H16   | 100061-77-9 | 50   |



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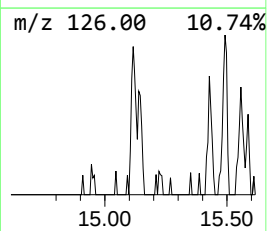
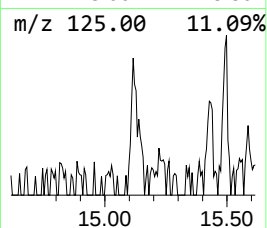
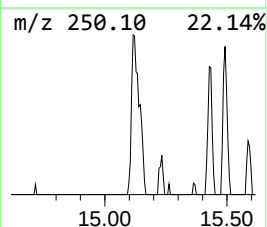
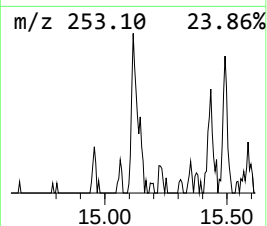
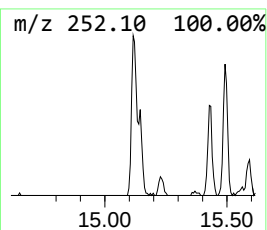
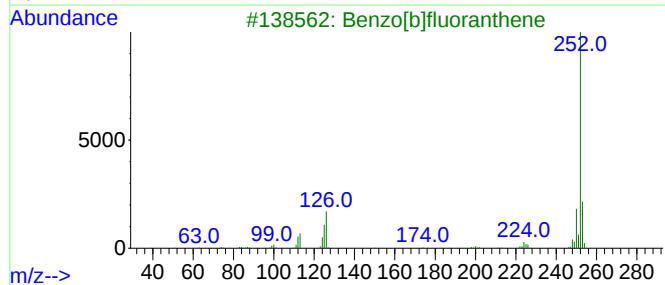
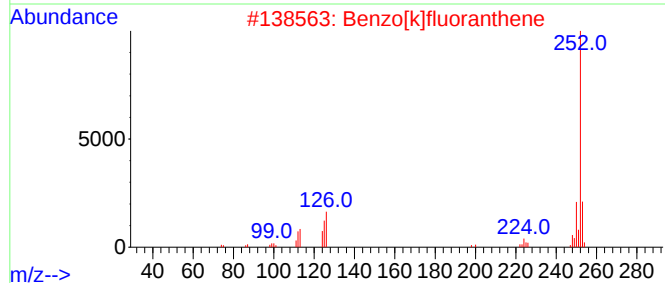
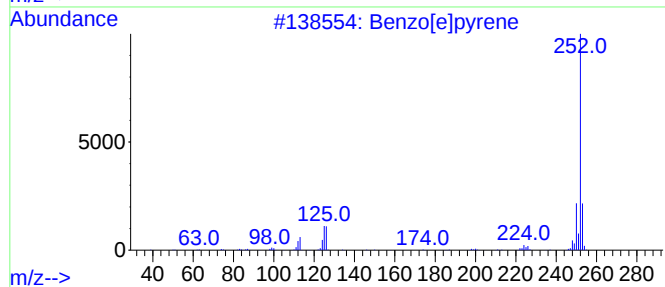
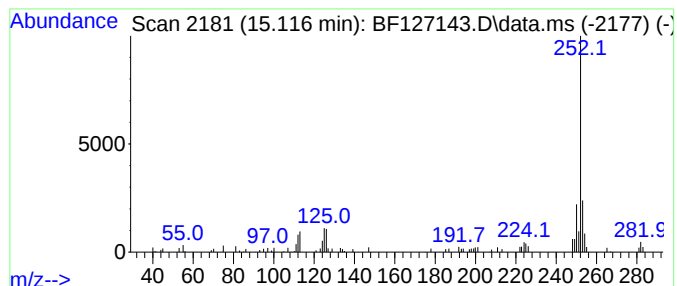
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Peak Number 4 Benzo[e]pyrene Concentration Rank 3

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 15.116 | 3.01 ng | 64304 | Perylene-d12     | 15.557 |

| Hit# | of | 5 | Tentative ID         | MW  | MolForm | CAS#        | Qual |
|------|----|---|----------------------|-----|---------|-------------|------|
| 1    |    |   | Benzo[e]pyrene       | 252 | C20H12  | 000192-97-2 | 94   |
| 2    |    |   | Benzo[k]fluoranthene | 252 | C20H12  | 000207-08-9 | 93   |
| 3    |    |   | Benzo[b]fluoranthene | 252 | C20H12  | 000205-99-2 | 89   |
| 4    |    |   | Benzo[a]pyrene       | 252 | C20H12  | 000050-32-8 | 89   |
| 5    |    |   | Perylene             | 252 | C20H12  | 000198-55-0 | 76   |



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TIC Library : C:\Database\NIST20.L  
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| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |        |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|--------|------|
|                    |        |         |       |          | #                     | RT     | Resp   | Conc |
| 2-Pentanone, 4-... | 5.116  | 2.0     | ng    | 54445    | 1                     | 6.887  | 544325 | 20.0 |
| Diethylene glyc... | 13.928 | 7.0     | ng    | 141763   | 5                     | 14.063 | 403188 | 20.0 |
| Supraene           | 14.910 | 4.4     | ng    | 94380    | 6                     | 15.557 | 427614 | 20.0 |
| Benzo[e]pyrene     | 15.116 | 3.0     | ng    | 64304    | 6                     | 15.557 | 427614 | 20.0 |