

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF042421\  
 Data File : BF123729.D  
 Acq On : 24 Apr 2021 21:30  
 Operator : JU/CG  
 Sample : M2152-06  
 Misc :  
 ALS Vial : 20 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 TP-4-COMP

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-BF041521.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123729.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         | 5.028       | 495           | 500         | 505          | rVB      | 147621         | 182921        | 3.31%           | 0.474%        |
| 2         | 5.440       | 566           | 570         | 573          | rBV      | 5991908        | 5196981       | 94.06%          | 13.475%       |
| 3         | 6.457       | 738           | 743         | 754          | rBV      | 5603558        | 5525093       | 100.00%         | 14.326%       |
| 4         | 6.822       | 801           | 805         | 808          | rBV      | 1692571        | 1402891       | 25.39%          | 3.638%        |
| 5         | 7.381       | 896           | 900         | 903          | rBV      | 3863238        | 3591582       | 65.00%          | 9.313%        |
| 6         | 8.104       | 1019          | 1023        | 1026         | rBV      | 2311934        | 1799371       | 32.57%          | 4.666%        |
| 7         | 9.180       | 1202          | 1206        | 1209         | rBV      | 6375575        | 5020449       | 90.87%          | 13.018%       |
| 8         | 9.263       | 1215          | 1220        | 1224         | rBV      | 95789          | 87826         | 1.59%           | 0.228%        |
| 9         | 9.575       | 1270          | 1273        | 1277         | rBV      | 163837         | 144353        | 2.61%           | 0.374%        |
| 10        | 9.857       | 1318          | 1321        | 1325         | rVB      | 2362855        | 1907483       | 34.52%          | 4.946%        |
| 11        | 10.645      | 1451          | 1455        | 1459         | rBV      | 3877738        | 3560383       | 64.44%          | 9.232%        |
| 12        | 11.345      | 1570          | 1574        | 1577         | rBV      | 2353178        | 1954395       | 35.37%          | 5.068%        |
| 13        | 11.416      | 1580          | 1586        | 1591         | rVB6     | 73369          | 103943        | 1.88%           | 0.270%        |
| 14        | 12.557      | 1777          | 1780        | 1783         | rBV      | 130056         | 110216        | 1.99%           | 0.286%        |
| 15        | 12.786      | 1816          | 1819        | 1821         | rVB      | 100946         | 77897         | 1.41%           | 0.202%        |
| 16        | 12.933      | 1840          | 1844        | 1847         | rBV      | 5044128        | 4184240       | 75.73%          | 10.849%       |
| 17        | 13.168      | 1881          | 1884        | 1889         | rBV6     | 47790          | 72742         | 1.32%           | 0.189%        |
| 18        | 13.474      | 1933          | 1936        | 1939         | rBV      | 124392         | 104341        | 1.89%           | 0.271%        |
| 19        | 13.845      | 1995          | 1999        | 2015         | rBV2     | 285007         | 598565        | 10.83%          | 1.552%        |
| 20        | 13.986      | 2019          | 2023        | 2026         | rBV      | 1570013        | 1313961       | 23.78%          | 3.407%        |
| 21        | 15.109      | 2211          | 2214        | 2219         | rVB2     | 80293          | 100291        | 1.82%           | 0.260%        |
| 22        | 15.451      | 2267          | 2272        | 2276         | rBV      | 987797         | 1225232       | 22.18%          | 3.177%        |
| 23        | 15.921      | 2348          | 2352        | 2358         | rBV3     | 78297          | 124608        | 2.26%           | 0.323%        |
| 24        | 17.251      | 2573          | 2578        | 2585         | rVB10    | 80342          | 176757        | 3.20%           | 0.458%        |

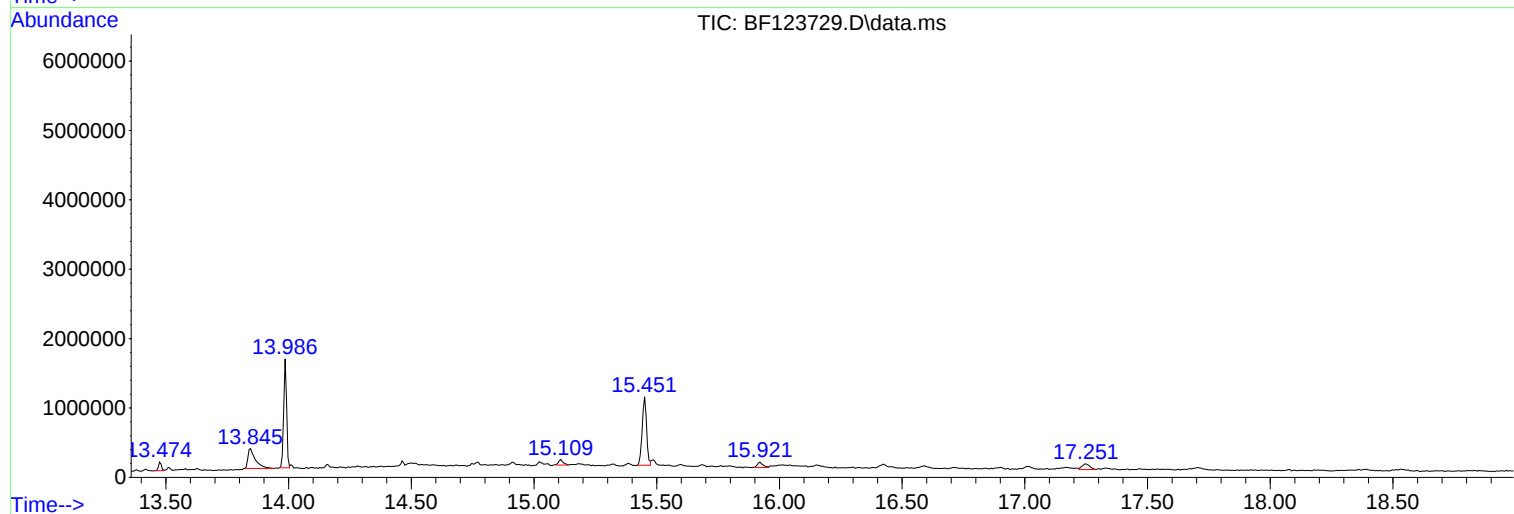
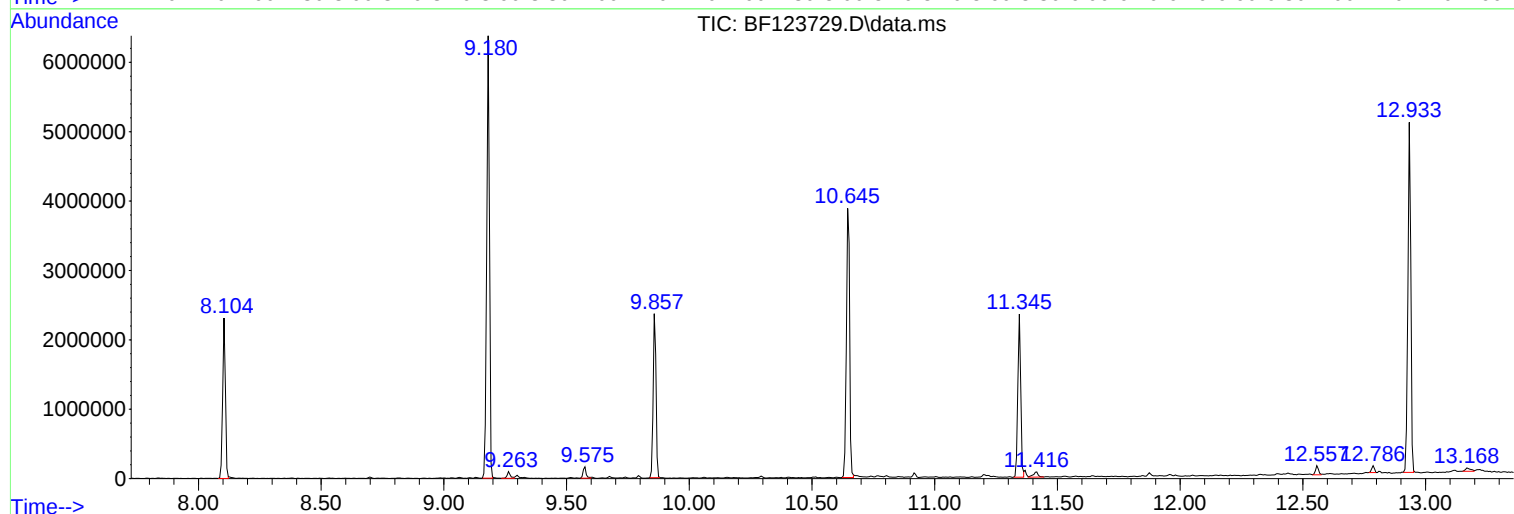
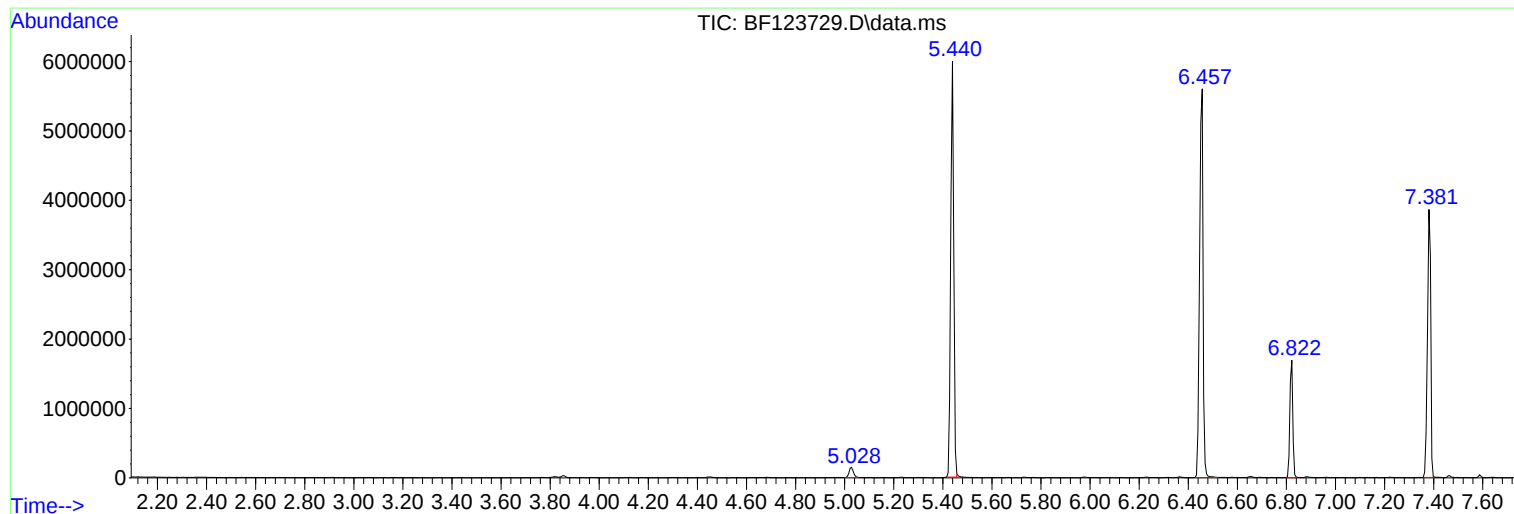
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ALS Vial : 20 Sample Multiplier: 1

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ClientSampleId :  
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF041521.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P



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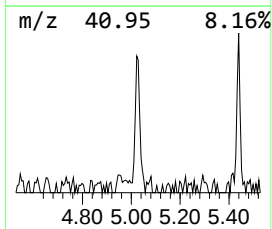
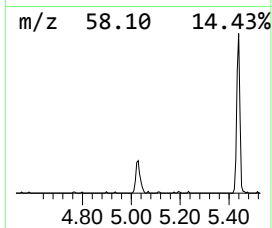
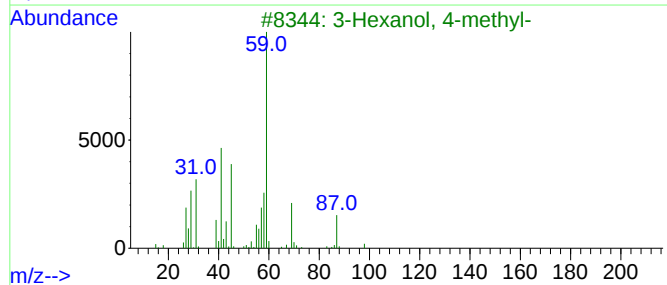
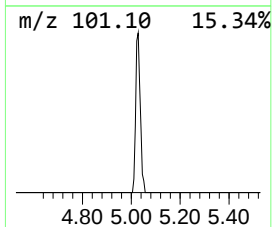
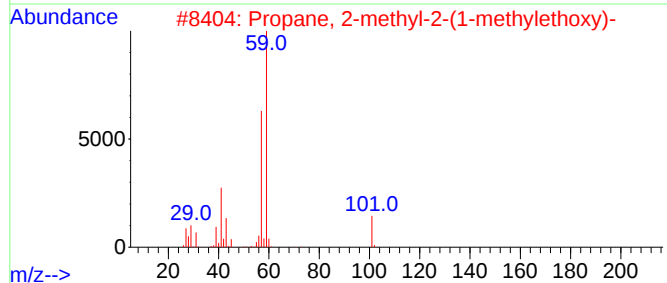
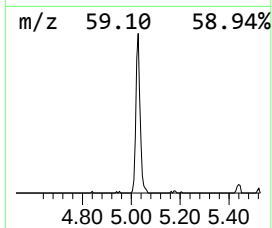
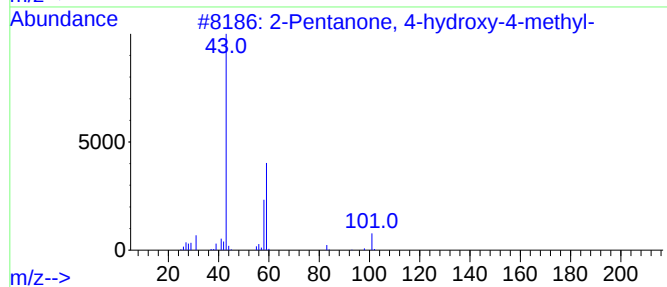
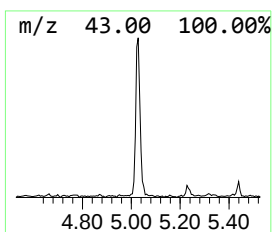
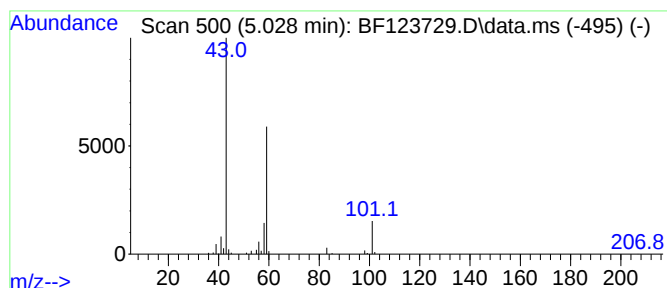
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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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.  |
|-------|---------|--------|------------------------|-------|
| 5.028 | 2.61 ng | 182921 | 1,4-Dichlorobenzene-d4 | 6.822 |

| Hit# | of                                  | 5   | Tentative ID | MW          | MolForm | CAS# | Qual |
|------|-------------------------------------|-----|--------------|-------------|---------|------|------|
| 1    | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2      | 000123-42-2 | 64      |      |      |
| 2    | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O       | 017348-59-3 | 33      |      |      |
| 3    | 3-Hexanol, 4-methyl-                | 116 | C7H16O       | 000615-29-2 | 9       |      |      |
| 4    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2      | 000540-88-5 | 9       |      |      |
| 5    | 2-Heptanone, 7,7-dichloro-          | 182 | C7H12Cl2O    | 066241-43-8 | 9       |      |      |



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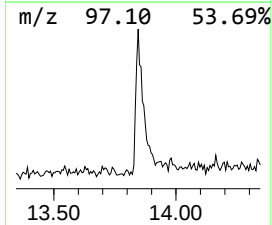
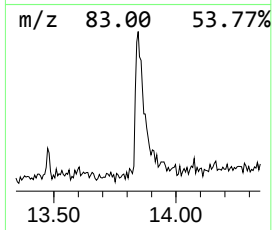
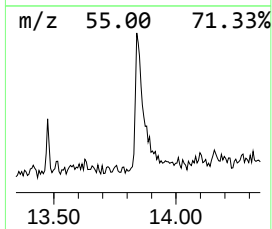
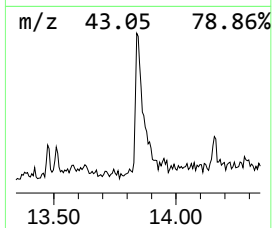
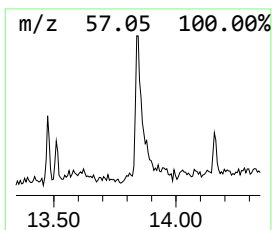
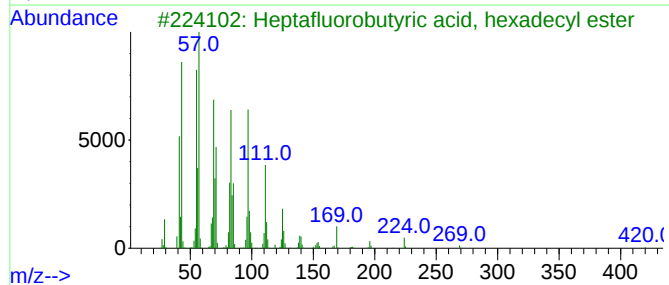
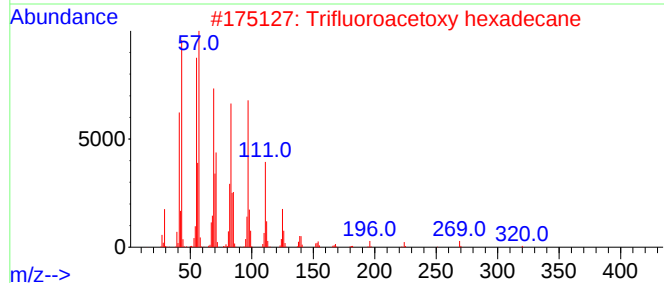
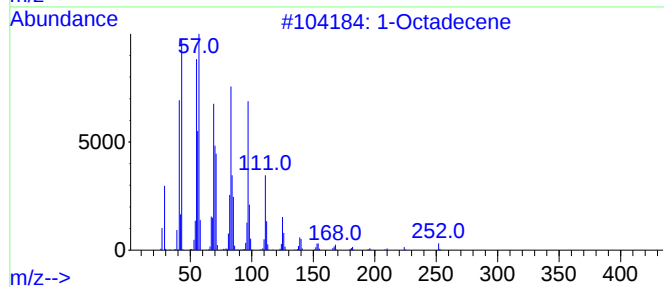
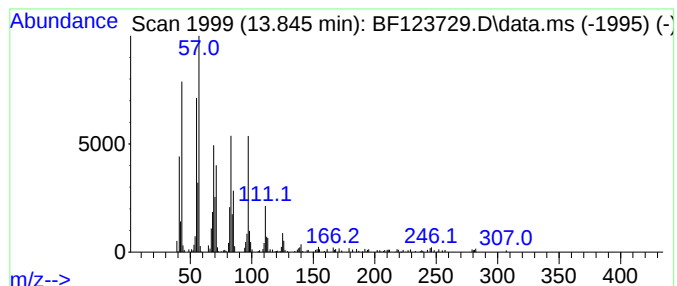
Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF041521.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 1-Octadecene Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.845 | 9.11 ng | 598565 | Chrysene-d12     | 13.986 |

| Hit# | of                                  | 5 | Tentative ID | MW  | MolForm    | CAS#        | Qual |
|------|-------------------------------------|---|--------------|-----|------------|-------------|------|
| 1    | 1-Octadecene                        |   |              | 252 | C18H36     | 000112-88-9 | 95   |
| 2    | Trifluoroacetoxy hexadecane         |   |              | 338 | C18H33F3O2 | 006222-03-3 | 91   |
| 3    | Heptafluorobutyric acid, hexadec... |   |              | 438 | C20H33F7O2 | 006385-15-5 | 91   |
| 4    | Pentafluoropropionic acid, hexad... |   |              | 388 | C19H33F5O2 | 006222-07-7 | 91   |
| 5    | Pentafluoropropionic acid, hepta... |   |              | 402 | C20H35F5O2 | 959218-78-1 | 91   |



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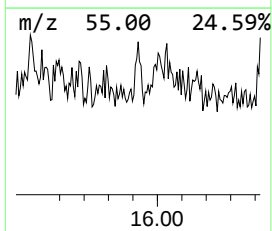
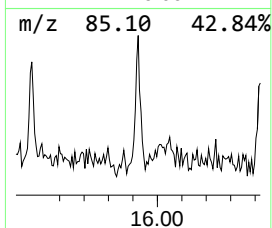
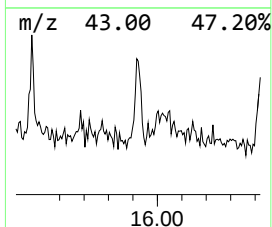
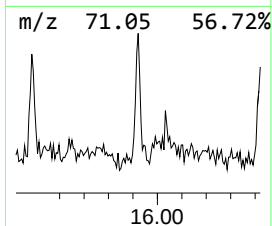
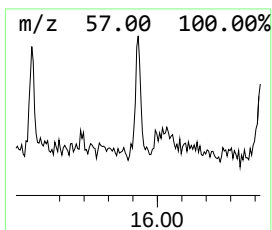
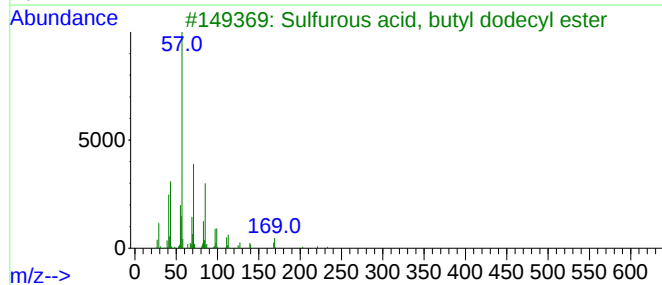
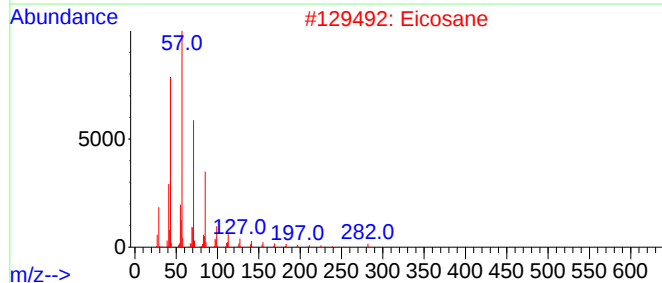
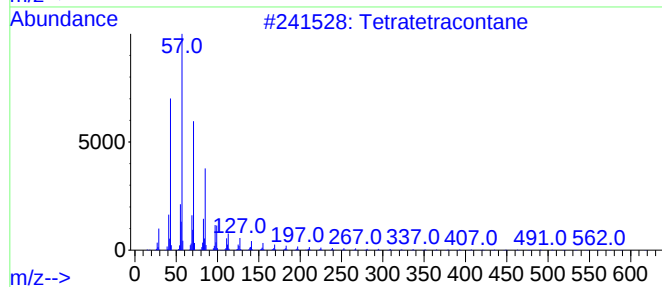
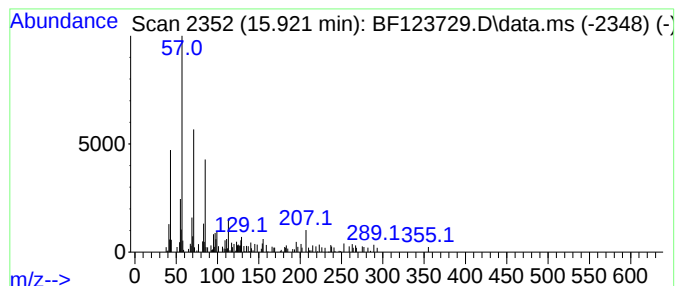
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Tetratetracontane Concentration Rank 4

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 15.921 | 2.03 ng | 124608 | Perylene-d12     | 15.451 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | Tetratetracontane                   | 619 | C44H90    | 007098-22-8  | 72   |
| 2    |    |   | Eicosane                            | 282 | C20H42    | 000112-95-8  | 72   |
| 3    |    |   | Sulfurous acid, butyl dodecyl ester | 306 | C16H34O3S | 1000309-17-9 | 72   |
| 4    |    |   | Hexadecane                          | 226 | C16H34    | 000544-76-3  | 72   |
| 5    |    |   | Hentriacontane                      | 437 | C31H64    | 000630-04-6  | 64   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF041521.M  
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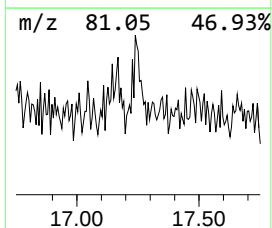
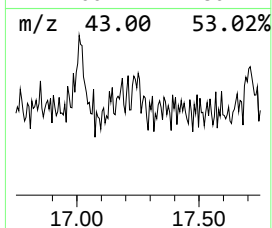
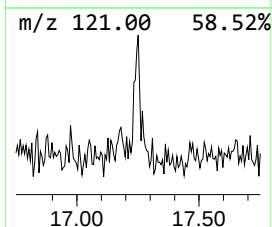
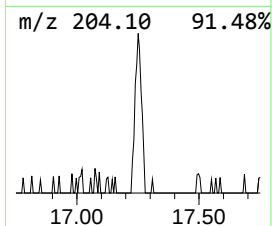
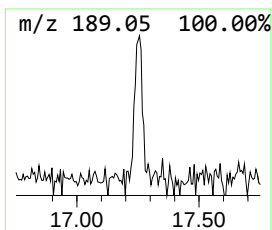
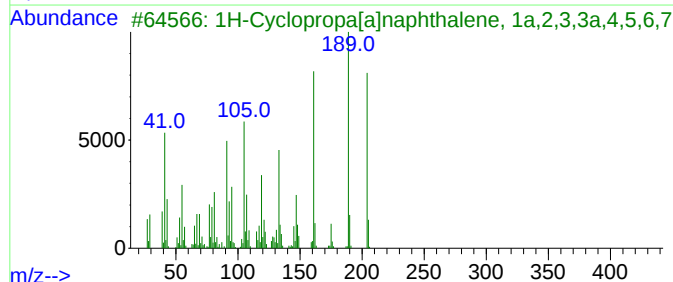
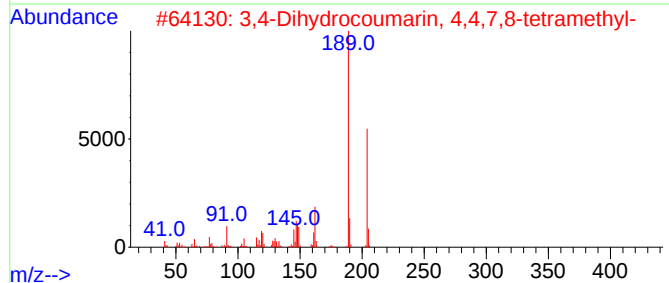
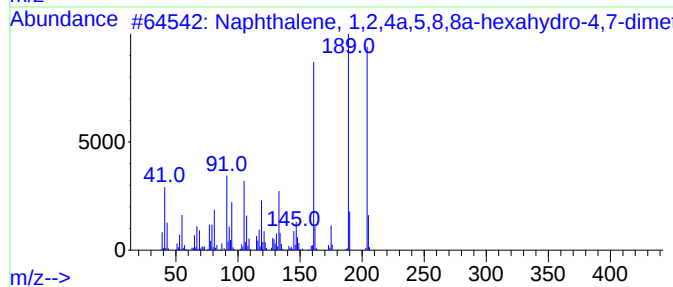
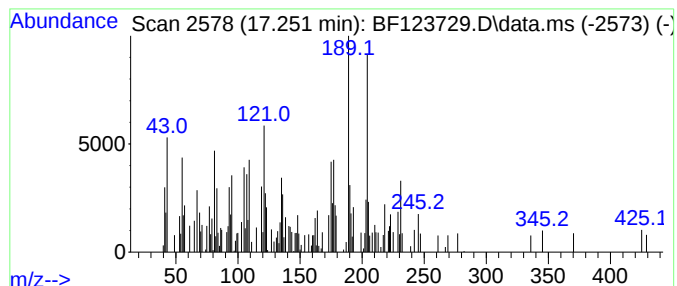
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Peak Number 4 unknown17.250 Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 17.250 | 2.89 ng | 176757 | Perylene-d12     | 15.451 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | Naphthalene, 1,2,4a,5,8,8a-hexah... | 204 | C15H24   | 005951-61-1 | 45   |
| 2    |    |   | 3,4-Dihydrocoumarin, 4,4,7,8-tet... | 204 | C13H16O2 | 040614-36-6 | 38   |
| 3    |    |   | 1H-Cyclopropa[a]naphthalene, 1a,... | 204 | C15H24   | 000489-29-2 | 38   |
| 4    |    |   | .delta.-Selinene                    | 204 | C15H24   | 028624-23-9 | 38   |
| 5    |    |   | Naphthalene, 2,3,4,4a,5,6-hexahy... | 204 | C15H24   | 000473-14-3 | 38   |



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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name   | RT     | EstConc | Units | Response | --Internal Standard-- |        |         |      |
|--------------------|--------|---------|-------|----------|-----------------------|--------|---------|------|
|                    |        |         |       |          | #                     | RT     | Resp    | Conc |
| 2-Pentanone, 4-... | 5.028  | 2.6     | ng    | 182921   | 1                     | 6.822  | 1402890 | 20.0 |
| 1-Octadecene       | 13.845 | 9.1     | ng    | 598565   | 5                     | 13.986 | 1313960 | 20.0 |
| Tetratetracontane  | 15.921 | 2.0     | ng    | 124608   | 6                     | 15.451 | 1225230 | 20.0 |
| unknown17.250      | 17.250 | 2.9     | ng    | 176757   | 6                     | 15.451 | 1225230 | 20.0 |