

Data Path : Z:\svoasrv\HPCHEM1\BNA\_F\Data\BF081623\  
 Data File : BF134809.D  
 Acq On : 16 Aug 2023 15:21  
 Operator : CG\JU  
 Sample : 04020-01  
 Misc :  
 ALS Vial : 15 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 E-2

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-BF080123.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134809.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         | 3.304       | 204           | 207         | 219          | rBV      | 34263          | 91877         | 3.20%           | 0.463%        |
| 2         | 5.428       | 564           | 568         | 572          | rBV      | 2518253        | 2610089       | 91.05%          | 13.155%       |
| 3         | 6.434       | 734           | 739         | 742          | rBV      | 2601957        | 2610783       | 91.07%          | 13.158%       |
| 4         | 6.628       | 768           | 772         | 783          | rBV      | 38470          | 50349         | 1.76%           | 0.254%        |
| 5         | 6.798       | 798           | 801         | 805          | rBV      | 1161391        | 922575        | 32.18%          | 4.650%        |
| 6         | 7.363       | 892           | 897         | 900          | rBV      | 1860818        | 1643249       | 57.32%          | 8.282%        |
| 7         | 8.081       | 1015          | 1019        | 1022         | rBV      | 1426118        | 1158047       | 40.40%          | 5.837%        |
| 8         | 9.157       | 1198          | 1202        | 1205         | rBV      | 3592548        | 2866755       | 100.00%         | 14.448%       |
| 9         | 9.275       | 1218          | 1222        | 1233         | rVB      | 71221          | 75743         | 2.64%           | 0.382%        |
| 10        | 9.833       | 1313          | 1317        | 1328         | rBV      | 1320918        | 1143791       | 39.90%          | 5.765%        |
| 11        | 10.622      | 1447          | 1451        | 1462         | rBV      | 1445274        | 1407330       | 49.09%          | 7.093%        |
| 12        | 11.322      | 1567          | 1570        | 1574         | rBV      | 996434         | 923113        | 32.20%          | 4.652%        |
| 13        | 11.857      | 1657          | 1661        | 1675         | rBV      | 170609         | 195745        | 6.83%           | 0.987%        |
| 14        | 12.645      | 1791          | 1795        | 1802         | rBV2     | 28356          | 40933         | 1.43%           | 0.206%        |
| 15        | 12.921      | 1837          | 1842        | 1845         | rBV      | 2645783        | 2443350       | 85.23%          | 12.314%       |
| 16        | 13.833      | 1993          | 1997        | 2003         | rBV2     | 90298          | 142210        | 4.96%           | 0.717%        |
| 17        | 13.974      | 2017          | 2021        | 2028         | rBV      | 821417         | 742891        | 25.91%          | 3.744%        |
| 18        | 14.745      | 2149          | 2152        | 2159         | rVB2     | 148032         | 186096        | 6.49%           | 0.938%        |
| 19        | 14.839      | 2165          | 2168        | 2172         | rVB      | 73434          | 70490         | 2.46%           | 0.355%        |
| 20        | 15.451      | 2267          | 2272        | 2278         | rBV      | 380966         | 515947        | 18.00%          | 2.600%        |

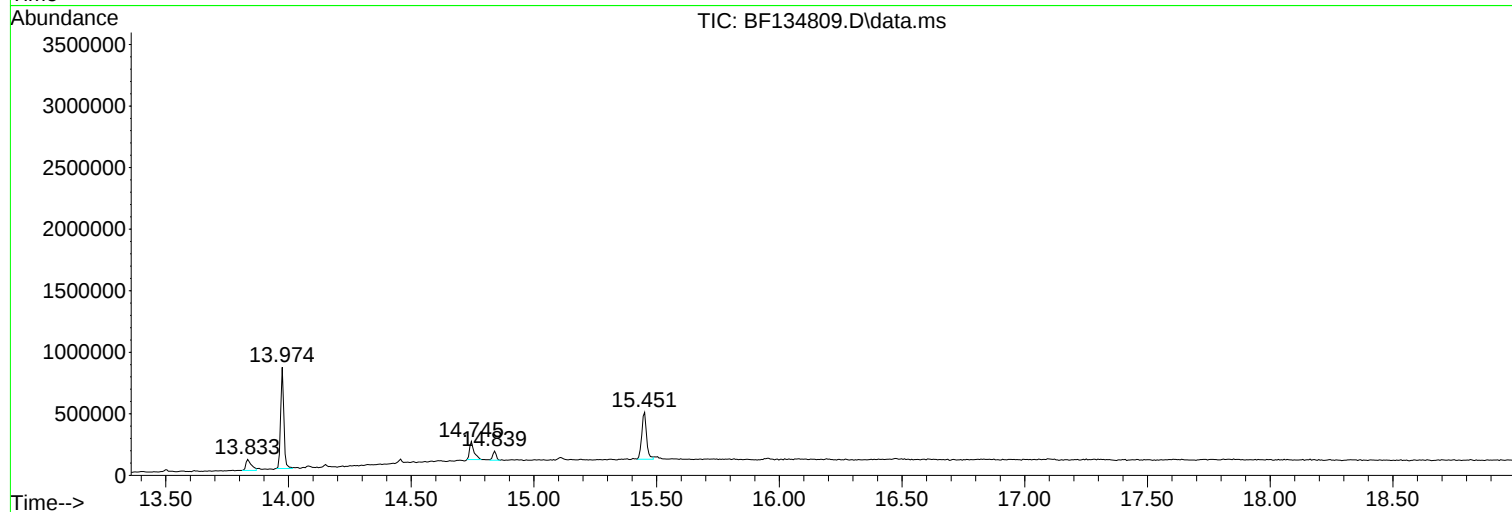
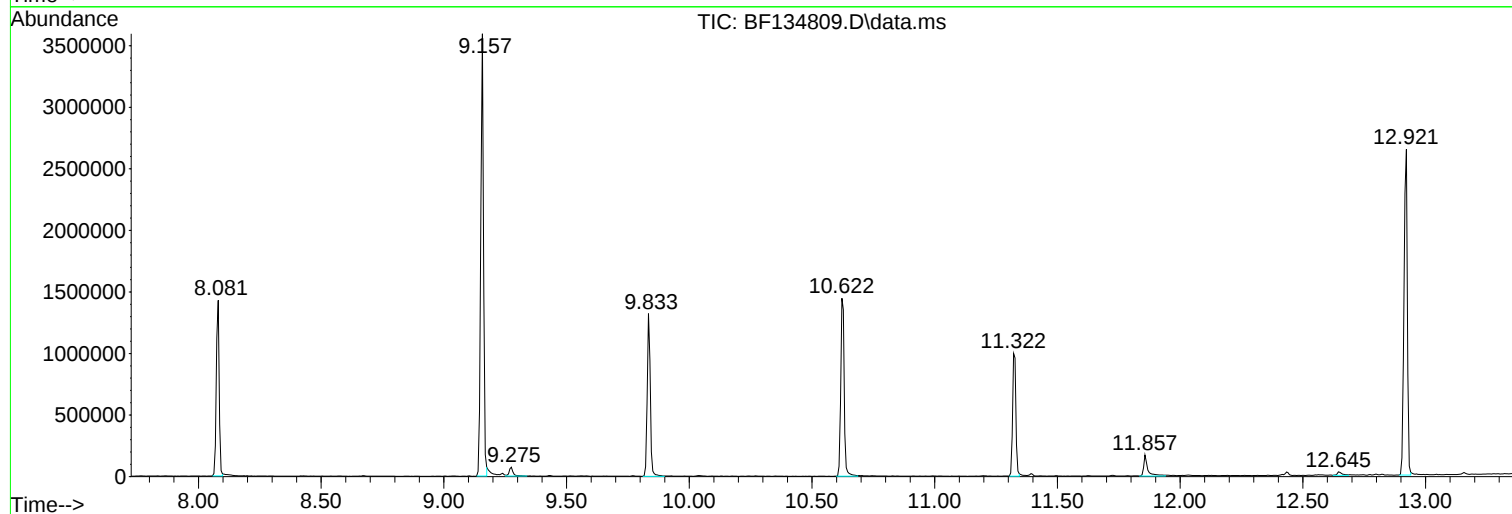
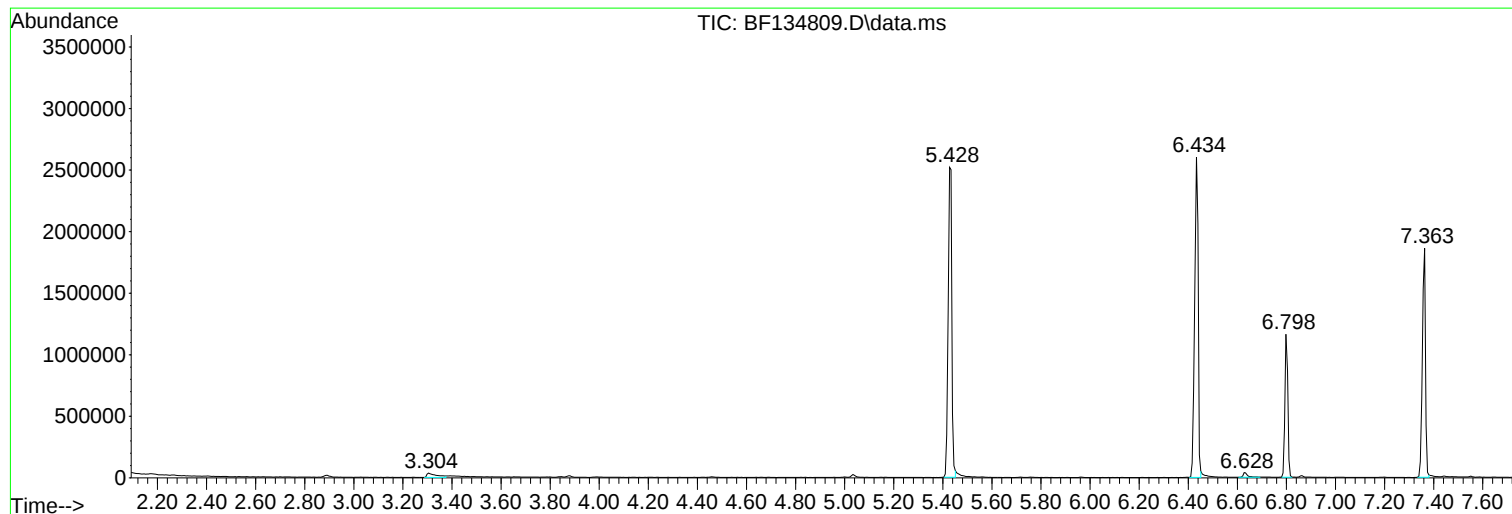
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ALS Vial : 15 Sample Multiplier: 1

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BNA\_F  
ClientSampleId :  
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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.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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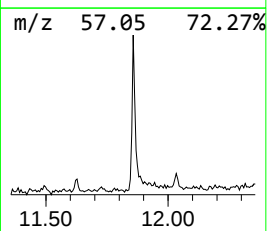
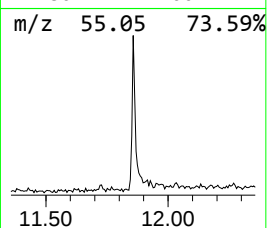
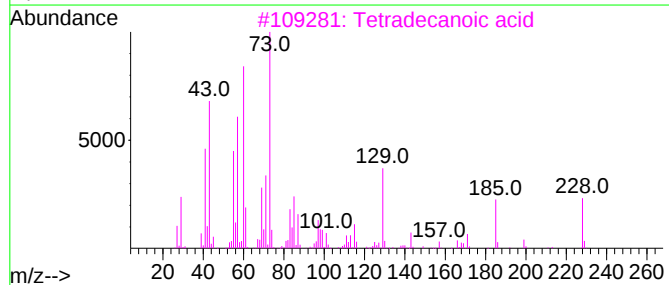
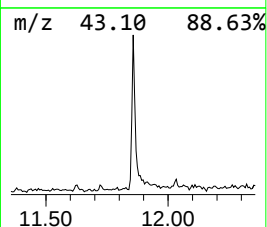
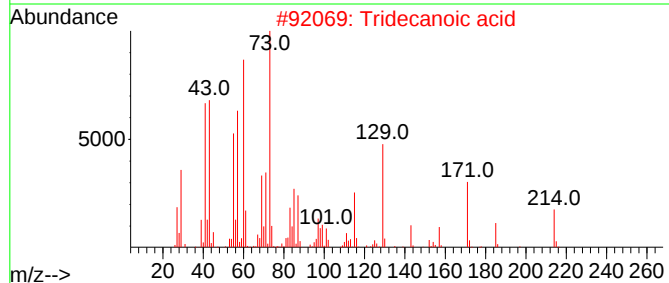
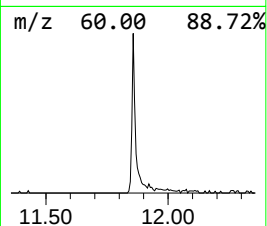
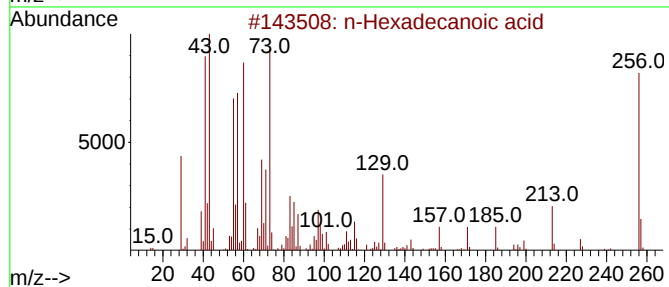
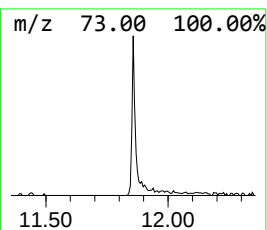
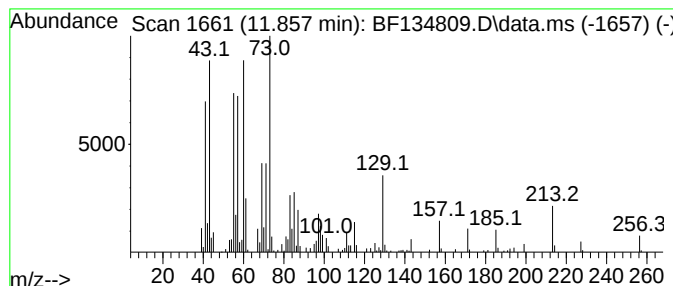
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 1 n-Hexadecanoic acid Concentration Rank 2

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 11.857 | 4.24 ng | 195745 | Phenanthrene-d10 | 11.322 |

| Hit# | of | 5 | Tentative ID          | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-----------------------|-----|----------|-------------|------|
| 1    |    |   | n-Hexadecanoic acid   | 256 | C16H32O2 | 000057-10-3 | 99   |
| 2    |    |   | Tridecanoic acid      | 214 | C13H26O2 | 000638-53-9 | 93   |
| 3    |    |   | Tetradecanoic acid    | 228 | C14H28O2 | 000544-63-8 | 91   |
| 4    |    |   | Pentadecanoic acid    | 242 | C15H30O2 | 001002-84-2 | 68   |
| 5    |    |   | 8-Methylnonanoic acid | 172 | C10H20O2 | 005963-14-4 | 60   |



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Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

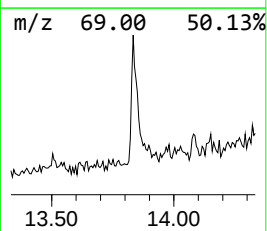
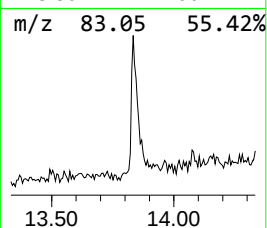
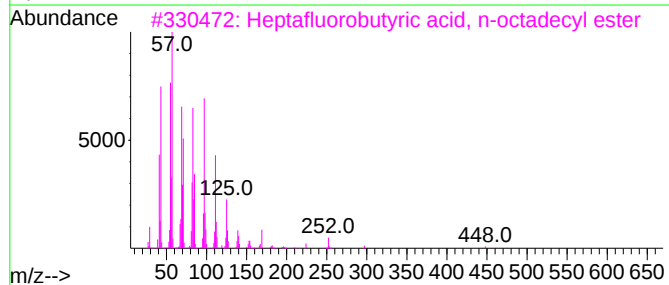
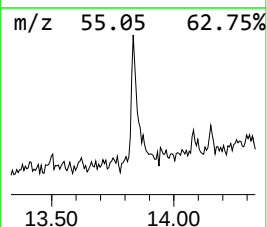
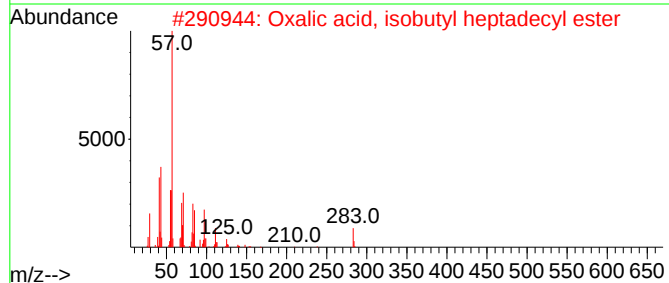
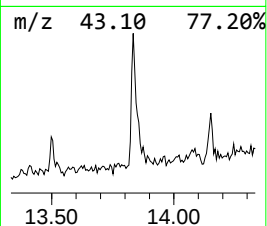
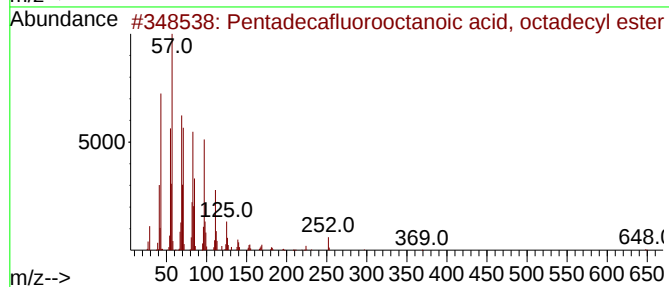
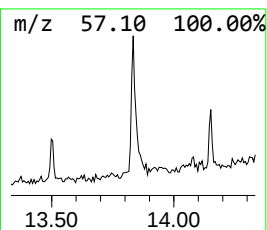
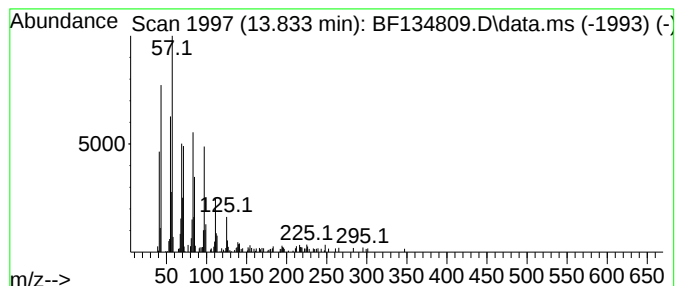
TIC Library : C:\Database\NIST20.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 Pentadecafluorooctanoic aci... Concentration Rank 3

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 13.833 | 3.83 ng | 142210 | Chrysene-d12     | 13.974 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-------------|--------------|------|
| 1    |    |   | Pentadecafluorooctanoic acid, oc... | 666 | C26H37F15O2 | 1000406-04-8 | 94   |
| 2    |    |   | Oxalic acid, isobutyl heptadecyl... | 384 | C23H44O4    | 1000309-38-2 | 91   |
| 3    |    |   | Heptafluorobutyric acid, n-octad... | 466 | C22H37F7O2  | 000400-57-7  | 91   |
| 4    |    |   | Methoxyacetic acid, heptadecyl e... | 328 | C20H40O3    | 1000282-99-1 | 91   |
| 5    |    |   | Oxalic acid, isobutyl octadecyl ... | 398 | C24H46O4    | 1000309-38-3 | 91   |



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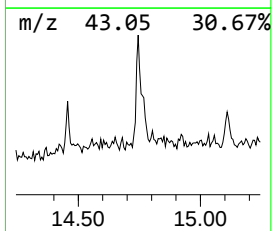
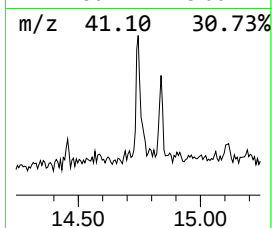
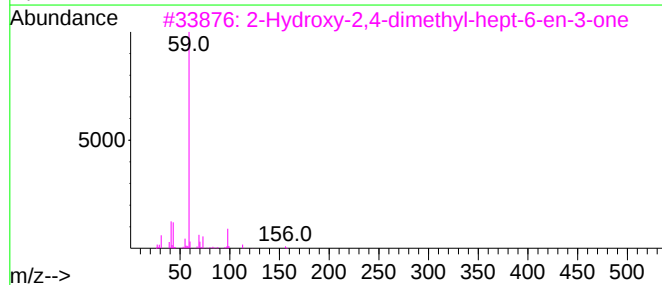
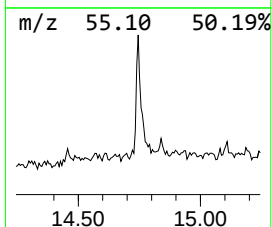
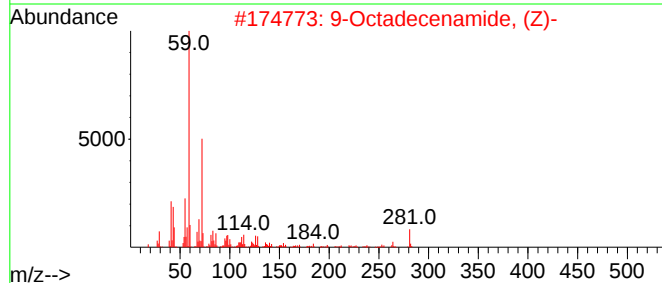
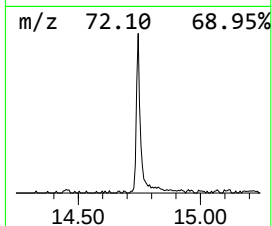
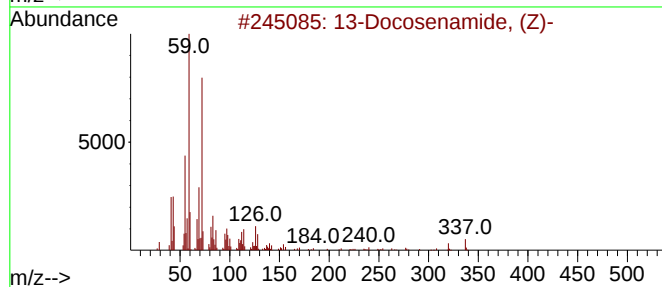
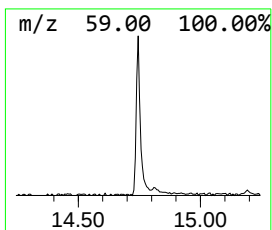
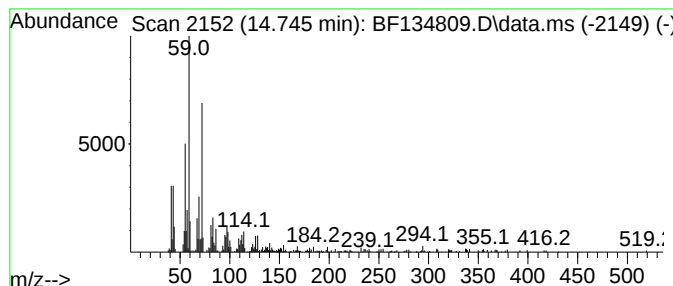
Quant Method : Z:\svoasrv\HPCHEM1\BNA\_F\Methods\8270-BF080123.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 3 13-Docosenamide, (Z)- Concentration Rank 1

| R.T.   | EstConc | Area   | Relative to ISTD | R.T.   |
|--------|---------|--------|------------------|--------|
| 14.745 | 7.21 ng | 186096 | Perylene-d12     | 15.451 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|----------|--------------|------|
| 1    |    |   | 13-Docosenamide, (Z)-               | 337 | C22H43NO | 000112-84-5  | 96   |
| 2    |    |   | 9-Octadecenamide, (Z)-              | 281 | C18H35NO | 000301-02-0  | 91   |
| 3    |    |   | 2-Hydroxy-2,4-dimethyl-hept-6-en... | 156 | C9H16O2  | 1000192-56-0 | 38   |
| 4    |    |   | Butanamide, 3-methyl-               | 101 | C5H11NO  | 000541-46-8  | 38   |
| 5    |    |   | Palmitoleamide                      | 253 | C16H31NO | 106010-22-4  | 27   |



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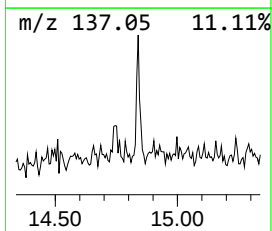
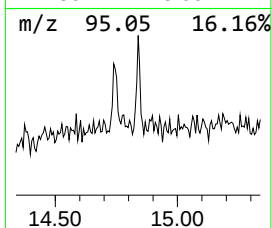
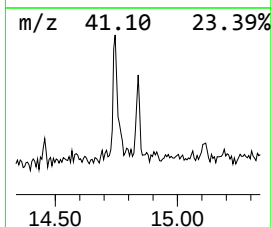
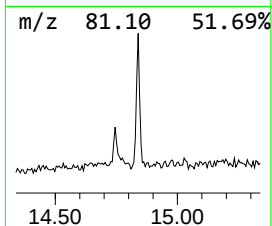
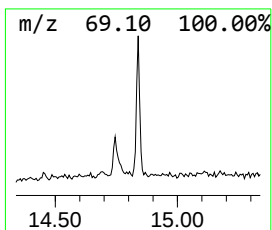
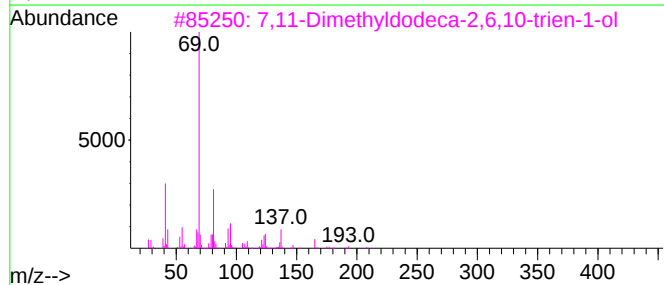
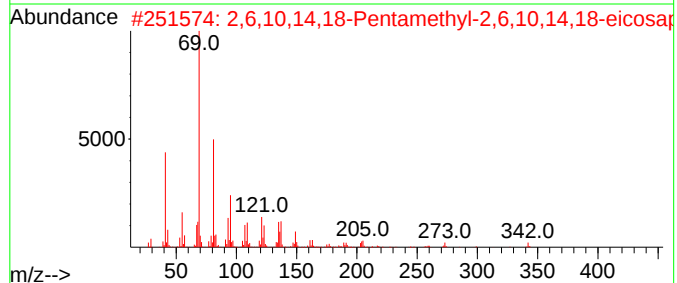
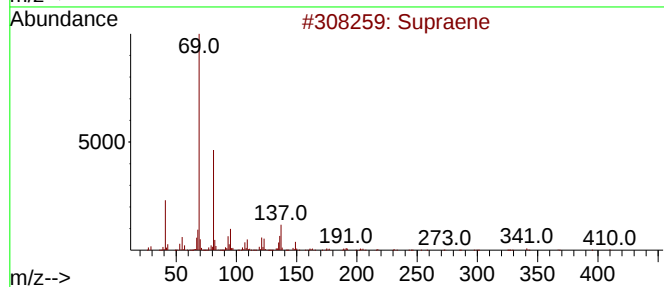
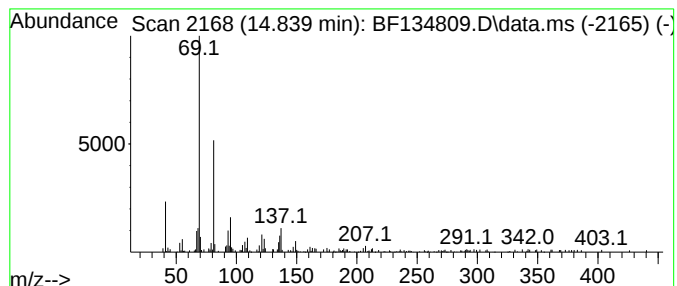
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Peak Number 4 Supraene Concentration Rank 4

| R.T.   | EstConc | Area  | Relative to ISTD | R.T.   |
|--------|---------|-------|------------------|--------|
| 14.839 | 2.73 ng | 70490 | Perylene-d12     | 15.451 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|---------|-------------|------|
| 1    |    |   | Supraene                            | 410 | C30H50  | 007683-64-9 | 83   |
| 2    |    |   | 2,6,10,14,18-Pentamethyl-2,6,10,... | 342 | C25H42  | 075581-03-2 | 83   |
| 3    |    |   | 7,11-Dimethyldodeca-2,6,10-trien... | 208 | C14H24O | 125529-10-4 | 72   |
| 4    |    |   | .psi.,.psi.-Carotene, 7,7',8,8',... | 547 | C40H66  | 000502-62-5 | 72   |
| 5    |    |   | 4,8,12-Tetradecatrienal, 5,9,13-... | 248 | C17H28O | 066408-55-7 | 72   |



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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 |
| n-Hexadecanoic ... | 11.857 | 4.2     | ng    | 195745   | 4                     | 11.322 | 923113 | 20.0 |
| Pentadecafluoro... | 13.833 | 3.8     | ng    | 142210   | 5                     | 13.974 | 742891 | 20.0 |
| 13-Docosenamide... | 14.745 | 7.2     | ng    | 186096   | 6                     | 15.451 | 515947 | 20.0 |
| Supraene           | 14.839 | 2.7     | ng    | 70490    | 6                     | 15.451 | 515947 | 20.0 |