

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\  
 Data File : BF107438.D  
 Acq On : 17 Jul 2018 10:12  
 Operator : JU/SJ  
 Sample : J3633-01  
 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 A-1(0-6)

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-BF071618.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| 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         | 5.219       | 484           | 490         | 495          | rBV      | 365353         | 410456        | 11.02%          | 1.131%        |
| 2         | 5.607       | 551           | 556         | 559          | rBV      | 3289360        | 3112789       | 83.58%          | 8.578%        |
| 3         | 6.607       | 720           | 726         | 729          | rBV      | 3314511        | 3358149       | 90.16%          | 9.254%        |
| 4         | 6.754       | 746           | 751         | 754          | rBV      | 3728795        | 3298738       | 88.57%          | 9.090%        |
| 5         | 6.984       | 786           | 790         | 793          | rBV      | 1197673        | 983742        | 26.41%          | 2.711%        |
| 6         | 7.136       | 812           | 816         | 820          | rBV      | 2691981        | 2466897       | 66.23%          | 6.798%        |
| 7         | 7.542       | 880           | 885         | 888          | rBV      | 2211528        | 2151875       | 57.78%          | 5.930%        |
| 8         | 8.266       | 1004          | 1008        | 1011         | rBV      | 1491616        | 1172292       | 31.48%          | 3.230%        |
| 9         | 9.342       | 1186          | 1191        | 1194         | rBV      | 3636879        | 3433327       | 92.18%          | 9.461%        |
| 10        | 9.442       | 1205          | 1208        | 1211         | rVB3     | 40137          | 41091         | 1.10%           | 0.113%        |
| 11        | 9.730       | 1253          | 1257        | 1260         | rBV      | 687143         | 548670        | 14.73%          | 1.512%        |
| 12        | 9.936       | 1288          | 1292        | 1297         | rVB6     | 44747          | 73247         | 1.97%           | 0.202%        |
| 13        | 10.025      | 1303          | 1307        | 1311         | rBV2     | 1612187        | 1400891       | 37.61%          | 3.860%        |
| 14        | 10.819      | 1437          | 1442        | 1445         | rBV      | 2666784        | 2515081       | 67.53%          | 6.931%        |
| 15        | 11.160      | 1496          | 1500        | 1504         | rVB4     | 57146          | 70515         | 1.89%           | 0.194%        |
| 16        | 11.195      | 1504          | 1506        | 1510         | rBV4     | 30375          | 40708         | 1.09%           | 0.112%        |
| 17        | 11.272      | 1515          | 1519        | 1523         | rVV7     | 37009          | 73957         | 1.99%           | 0.204%        |
| 18        | 11.330      | 1525          | 1529        | 1532         | rVV5     | 25944          | 40023         | 1.07%           | 0.110%        |
| 19        | 11.519      | 1557          | 1561        | 1564         | rBV      | 1850202        | 1553647       | 41.71%          | 4.281%        |
| 20        | 11.683      | 1585          | 1589        | 1592         | rBV6     | 33797          | 47917         | 1.29%           | 0.132%        |
| 21        | 11.960      | 1633          | 1636        | 1639         | rBV5     | 31882          | 38339         | 1.03%           | 0.106%        |
| 22        | 12.024      | 1643          | 1647        | 1652         | rBV3     | 258669         | 307957        | 8.27%           | 0.849%        |
| 23        | 12.160      | 1660          | 1670        | 1672         | rBV8     | 144982         | 368702        | 9.90%           | 1.016%        |
| 24        | 12.477      | 1721          | 1724        | 1730         | rVB8     | 22975          | 43650         | 1.17%           | 0.120%        |
| 25        | 12.542      | 1731          | 1735        | 1737         | rVV3     | 85271          | 81269         | 2.18%           | 0.224%        |
| 26        | 12.583      | 1737          | 1742        | 1745         | rVV7     | 52143          | 73652         | 1.98%           | 0.203%        |
| 27        | 12.813      | 1778          | 1781        | 1786         | rBV6     | 47441          | 75838         | 2.04%           | 0.209%        |
| 28        | 12.907      | 1795          | 1797        | 1801         | rVB4     | 86743          | 81745         | 2.19%           | 0.225%        |
| 29        | 12.983      | 1808          | 1810        | 1813         | rBV4     | 56142          | 50194         | 1.35%           | 0.138%        |
| 30        | 13.107      | 1826          | 1831        | 1834         | rBV      | 3914646        | 3724505       | 100.00%         | 10.264%       |
| 31        | 13.295      | 1858          | 1863        | 1864         | rBV5     | 38785          | 54576         | 1.47%           | 0.150%        |
| 32        | 13.318      | 1865          | 1867        | 1870         | rVB4     | 62661          | 56186         | 1.51%           | 0.155%        |
| 33        | 13.377      | 1873          | 1877        | 1879         | rBV4     | 40484          | 61289         | 1.65%           | 0.169%        |
| 34        | 13.565      | 1905          | 1909        | 1913         | rBV7     | 43386          | 71585         | 1.92%           | 0.197%        |

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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-1(0-6)

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-BF071618.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 35 | 13.618 | 1915 | 1918 | 1920 | rBV4 | 50295   | 49892   | 1.34%  | 0.137% |
| 36 | 13.665 | 1920 | 1926 | 1927 | rVV6 | 79976   | 118084  | 3.17%  | 0.325% |
| 37 | 13.683 | 1927 | 1929 | 1934 | rVB6 | 69065   | 89878   | 2.41%  | 0.248% |
| 38 | 13.983 | 1976 | 1980 | 1984 | rBV3 | 338741  | 385035  | 10.34% | 1.061% |
| 39 | 14.165 | 2007 | 2011 | 2014 | rBV  | 1598968 | 1388250 | 37.27% | 3.826% |
| 40 | 14.307 | 2032 | 2035 | 2039 | rVB2 | 127979  | 133744  | 3.59%  | 0.369% |
| 41 | 14.612 | 2084 | 2087 | 2091 | rBV2 | 146259  | 163860  | 4.40%  | 0.452% |
| 42 | 14.936 | 2140 | 2142 | 2145 | rVB4 | 97507   | 98501   | 2.64%  | 0.271% |
| 43 | 15.018 | 2153 | 2156 | 2159 | rVB2 | 110406  | 111591  | 3.00%  | 0.308% |
| 44 | 15.065 | 2159 | 2164 | 2169 | rBV8 | 251579  | 433600  | 11.64% | 1.195% |
| 45 | 15.301 | 2201 | 2204 | 2207 | rBV5 | 89791   | 108626  | 2.92%  | 0.299% |
| 46 | 15.701 | 2267 | 2272 | 2278 | rVB2 | 905568  | 1264047 | 33.94% | 3.483% |
| 47 | 18.871 | 2809 | 2811 | 2815 | rBV5 | 43119   | 60157   | 1.62%  | 0.166% |

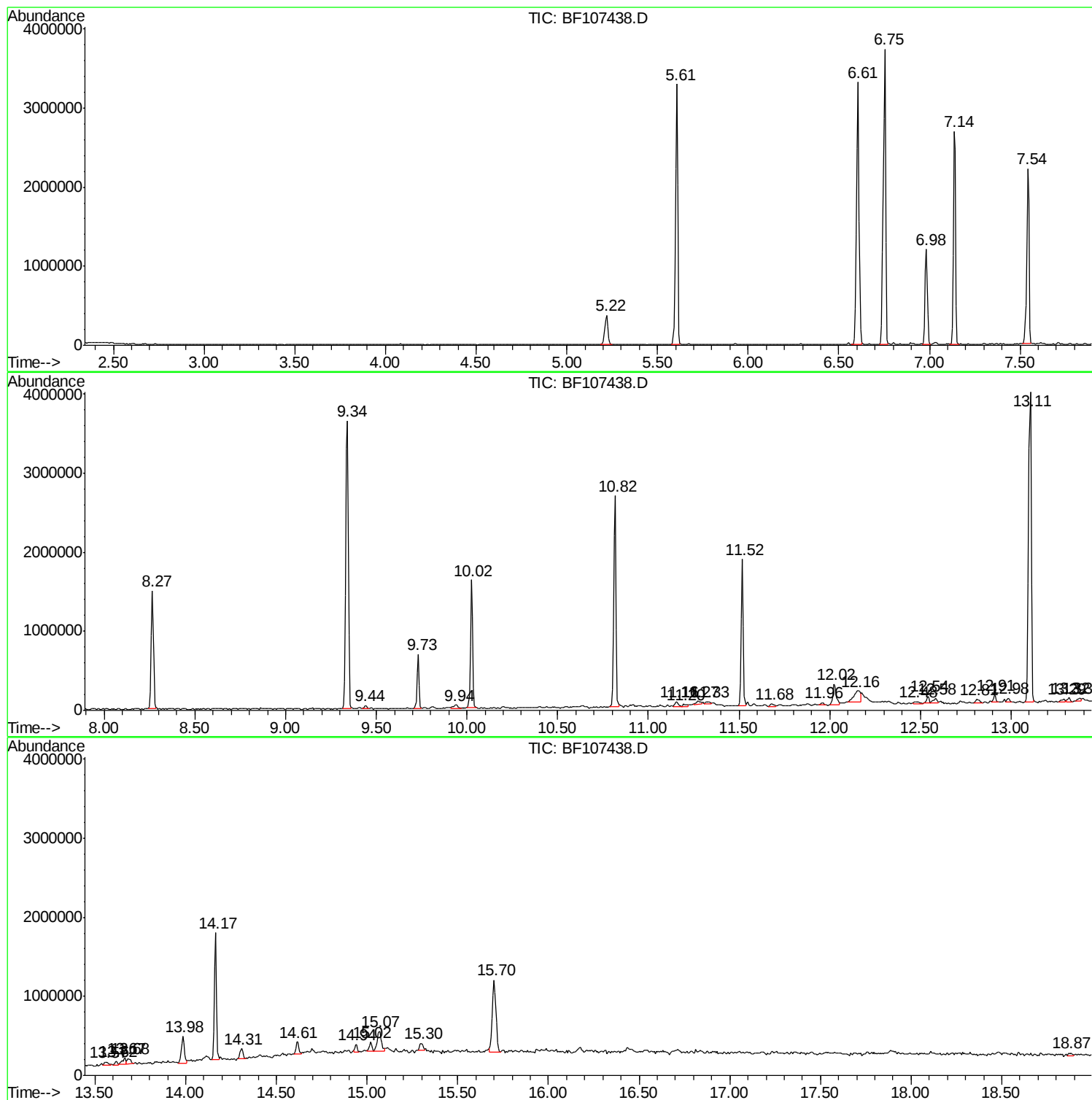
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Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampled :  
A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\  
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 Misc :  
 ALS Vial : 3 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

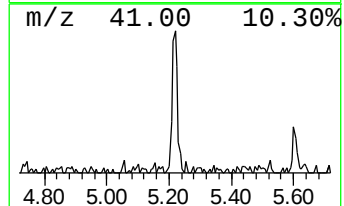
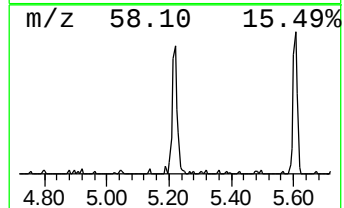
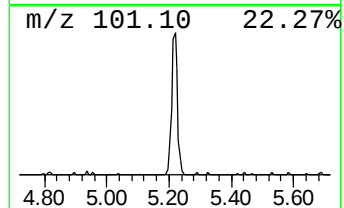
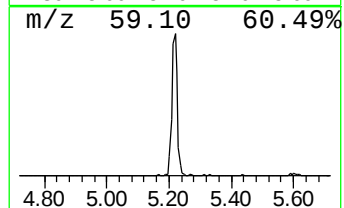
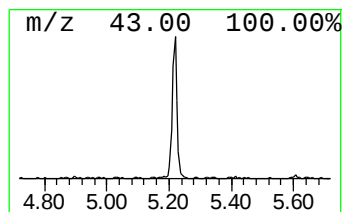
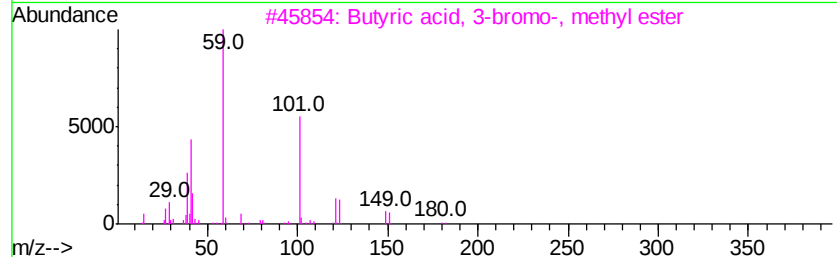
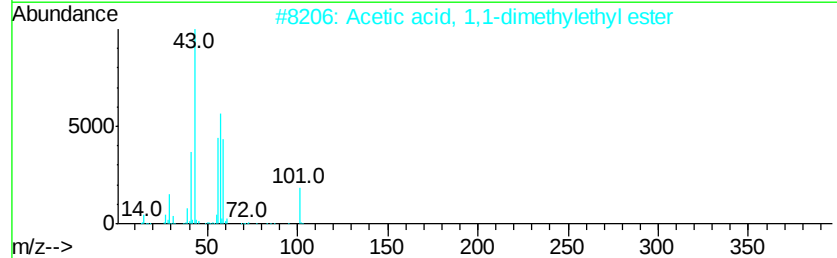
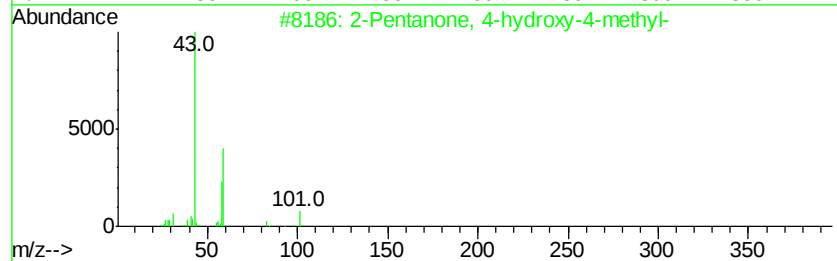
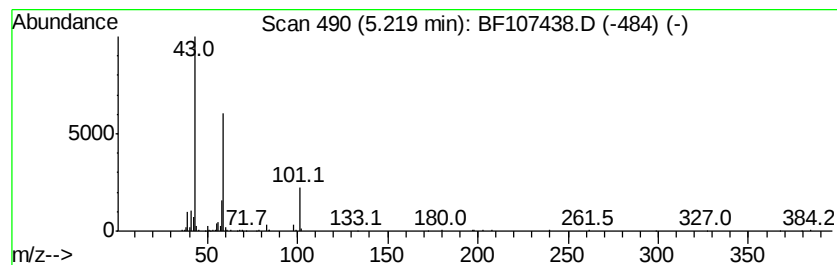
TIC Library : C:\DATABASE\NIST11.L  
 TIC Integration Parameters: LSCINT.P

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 Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 5.22 | 8.34 ng | 410456 | 1,4-Dichlorobenzene-d4 | 6.98 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 38   |
| 3    |    |   | Butyric acid, 3-bromo-, methyl e... | 180 | C5H9BrO2 | 021249-59-2 | 37   |
| 4    |    |   | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 35   |
| 5    |    |   | Dimethadione                        | 129 | C5H7NO3  | 000695-53-4 | 33   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

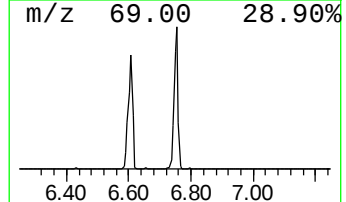
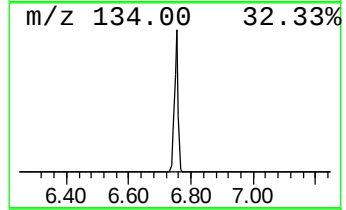
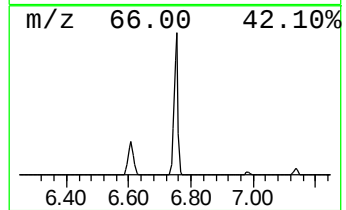
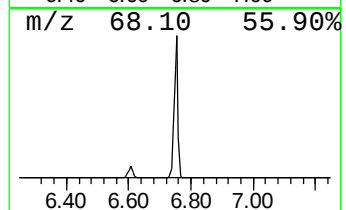
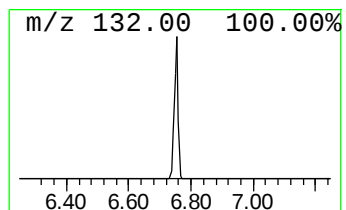
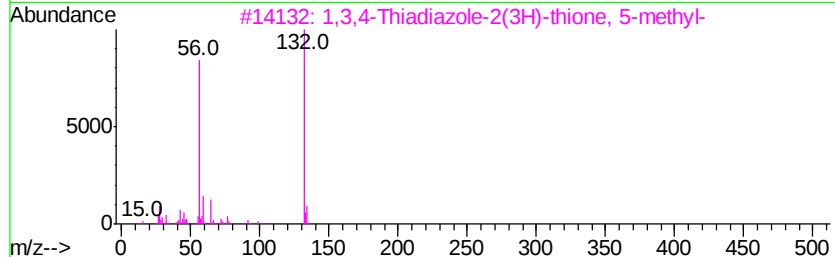
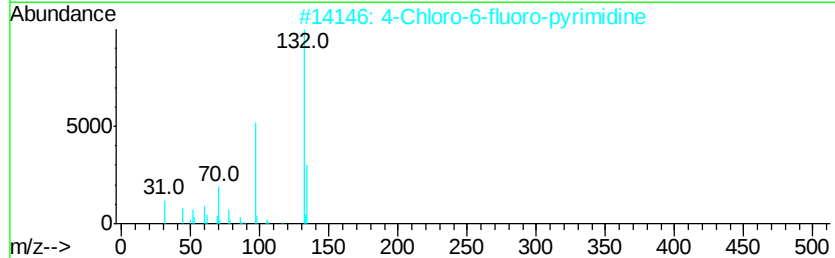
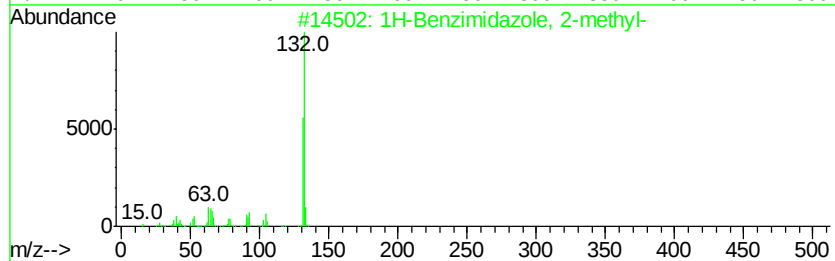
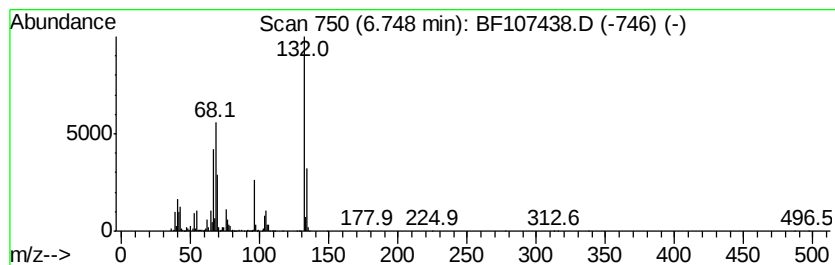
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 2 unknown6.75 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.75 | 67.07 ng | 3298740 | 1,4-Dichlorobenzene-d4 | 6.98 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 1H-Benzimidazole, 2-methyl-         | 132 | C8H8N2    | 000615-15-6  | 14   |
| 2    |    | 4-Chloro-6-fluoro-pyrimidine        | 132 | C4H2ClFN2 | 051422-01-6  | 14   |
| 3    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 14   |
| 4    |    | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 10   |
| 5    |    | Tranylcypromine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

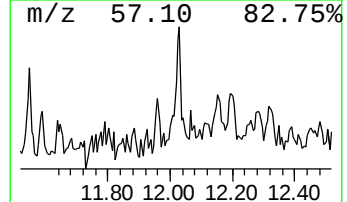
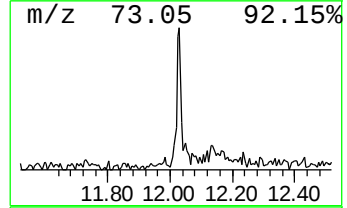
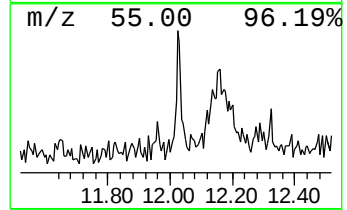
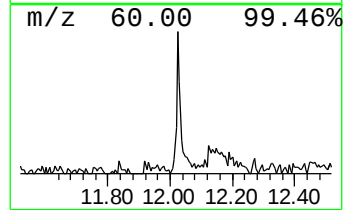
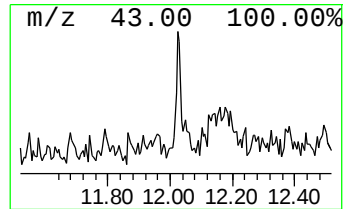
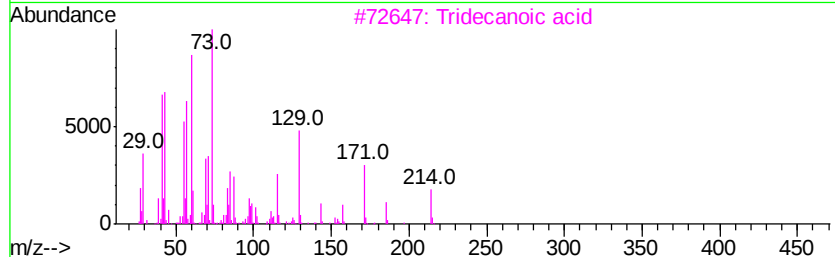
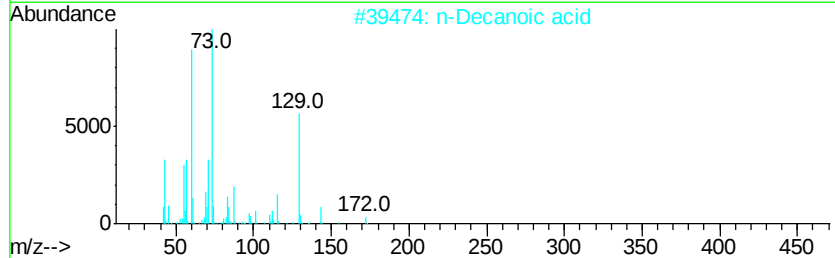
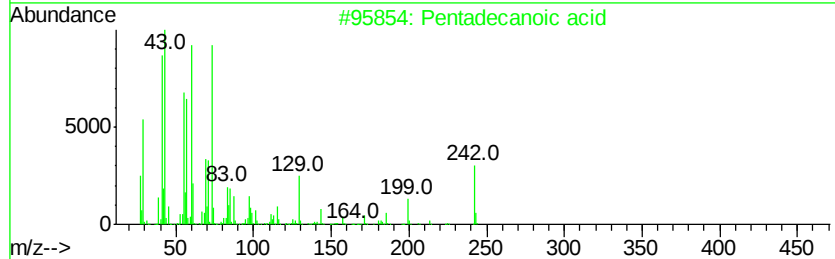
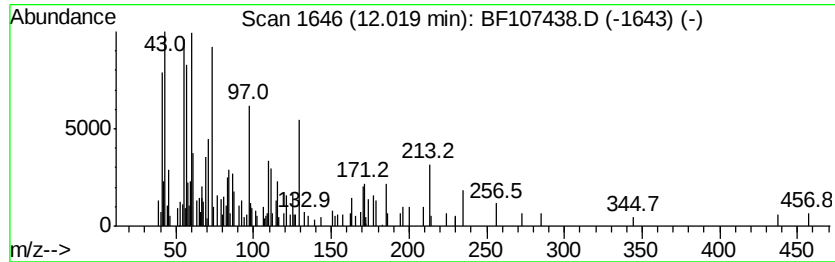
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 4 Pentadecanoic acid Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.02 | 3.96 ng | 307957 | Phenanthrene-d10 | 11.52 |

| Hit# of | 5 | Tentative ID            | MW  | MolForm    | CAS#        | Qual |
|---------|---|-------------------------|-----|------------|-------------|------|
| 1       |   | Pentadecanoic acid      | 242 | C15H30O2   | 001002-84-2 | 74   |
| 2       |   | n-Decanoic acid         | 172 | C10H20O2   | 000334-48-5 | 70   |
| 3       |   | Tridecanoic acid        | 214 | C13H26O2   | 000638-53-9 | 70   |
| 4       |   | n-Hexadecanoic acid     | 256 | C16H32O2   | 000057-10-3 | 55   |
| 5       |   | 11-Bromoundecanoic acid | 264 | C11H21BrO2 | 002834-05-1 | 47   |



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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

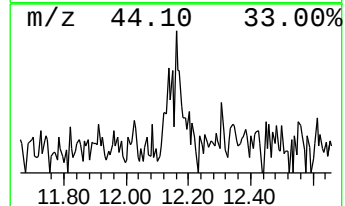
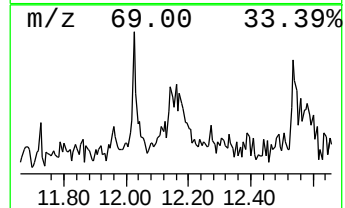
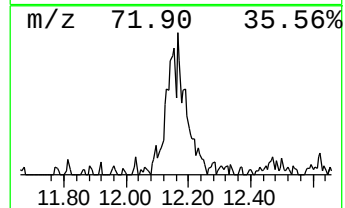
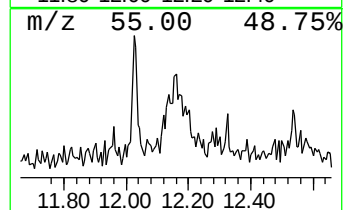
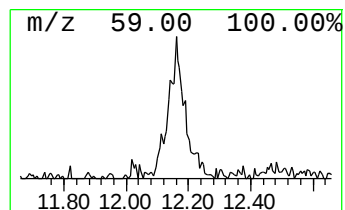
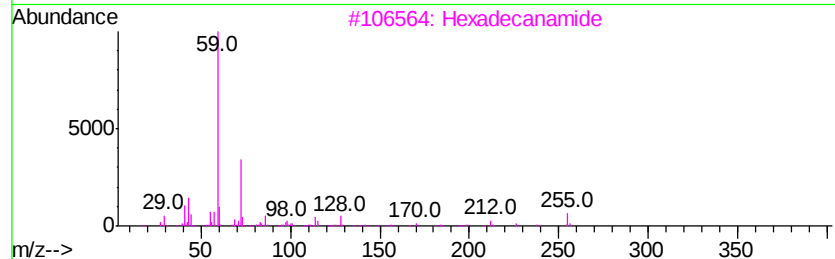
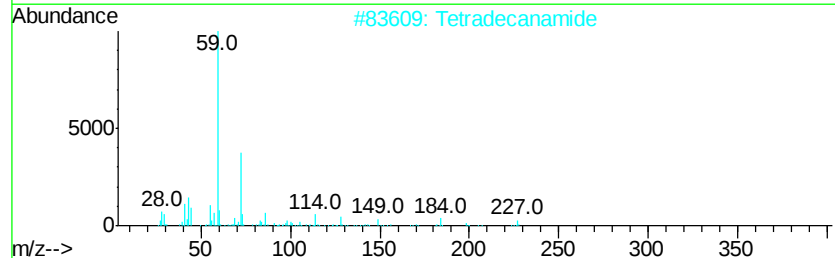
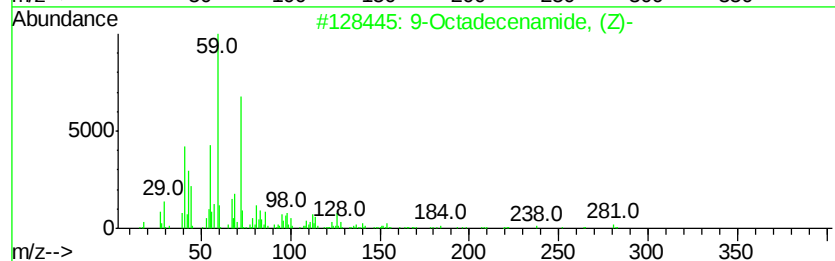
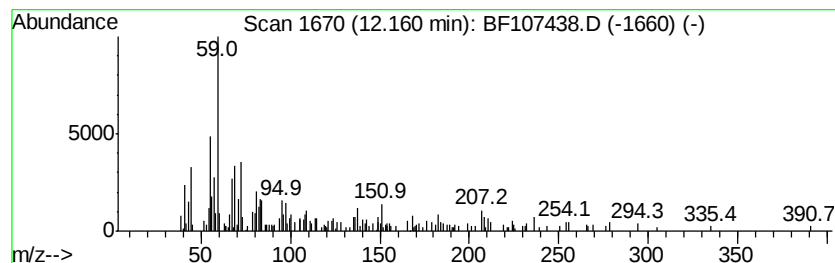
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 5 9-Octadecenamide, (Z)- Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.16 | 4.75 ng | 368702 | Phenanthrene-d10 | 11.52 |

| Hit# of | 5 | Tentative ID           | MW  | MolForm  | CAS#        | Qual |
|---------|---|------------------------|-----|----------|-------------|------|
| 1       |   | 9-Octadecenamide, (Z)- | 281 | C18H35NO | 000301-02-0 | 53   |
| 2       |   | Tetradecanamide        | 227 | C14H29NO | 000638-58-4 | 53   |
| 3       |   | Hexadecanamide         | 255 | C16H33NO | 000629-54-9 | 53   |
| 4       |   | 4-Cyclohexylbutyramide | 169 | C10H19NO | 004441-62-7 | 53   |
| 5       |   | Allyldimethylsilane    | 100 | C5H12Si  | 003937-30-2 | 50   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\  
Data File : BF107438.D  
Acq On : 17 Jul 2018 10:12  
Operator : JU/SJ  
Sample : J3633-01  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

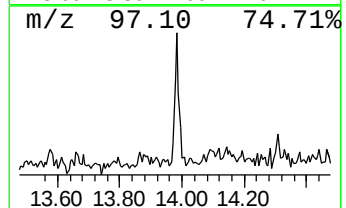
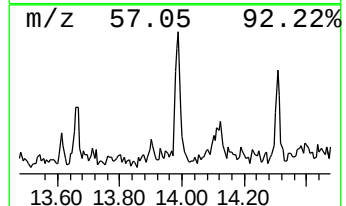
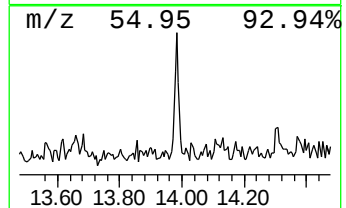
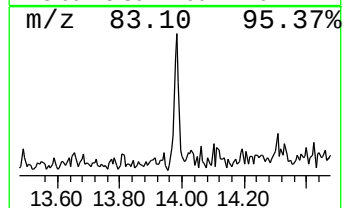
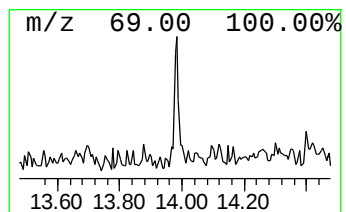
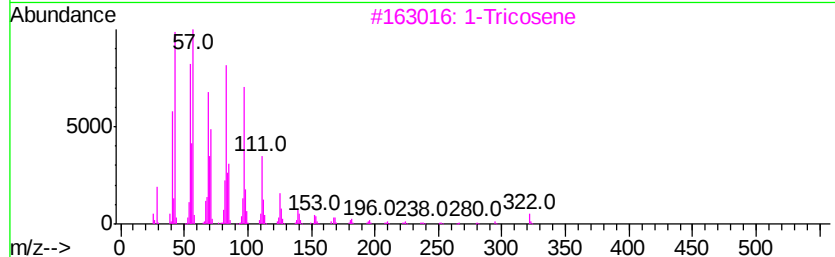
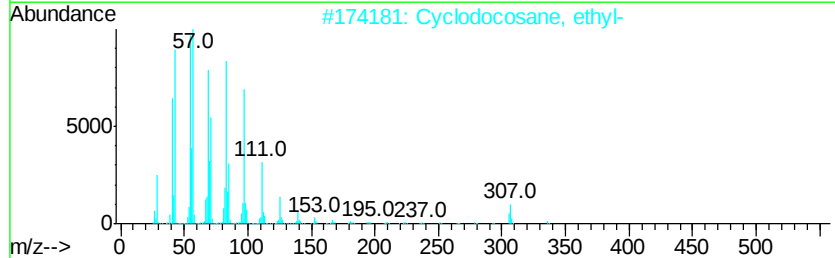
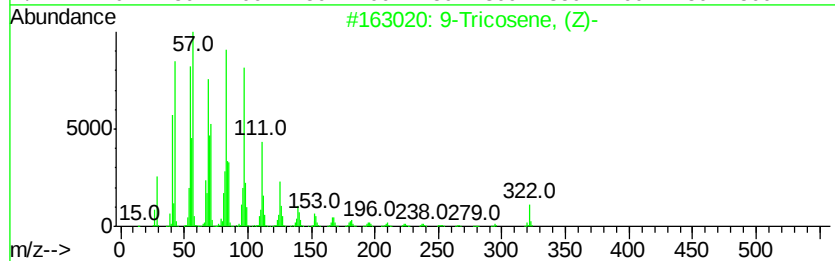
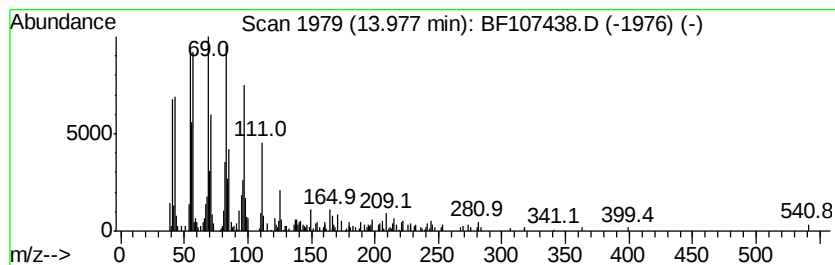
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 9-Tricosene, (Z)- Concentration Rank 5

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.98 | 5.55 ng | 385035 | Chrysene-d12     | 14.17 |

| Hit# of | 5 | Tentative ID          | MW  | MolForm | CAS#         | Qual |
|---------|---|-----------------------|-----|---------|--------------|------|
| 1       |   | 9-Tricosene, (Z)-     | 322 | C23H46  | 027519-02-4  | 95   |
| 2       |   | Cyclodocosane, ethyl- | 336 | C24H48  | 1000151-22-6 | 95   |
| 3       |   | 1-Tricosene           | 322 | C23H46  | 018835-32-0  | 93   |
| 4       |   | 2-Methyl-2-docosene   | 322 | C23H46  | 1000131-16-9 | 91   |
| 5       |   | E-7-Octadecene        | 252 | C18H36  | 1000130-92-0 | 86   |



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Data File : BF107438.D  
Acq On : 17 Jul 2018 10:12  
Operator : JU/SJ  
Sample : J3633-01  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

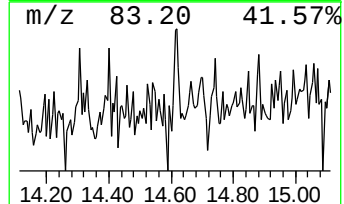
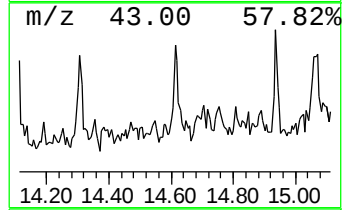
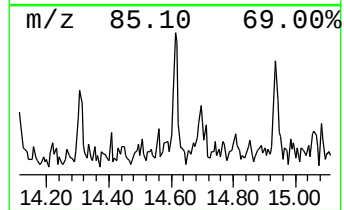
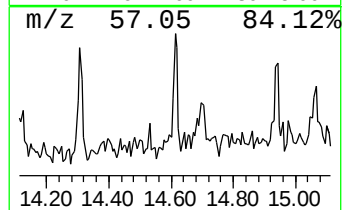
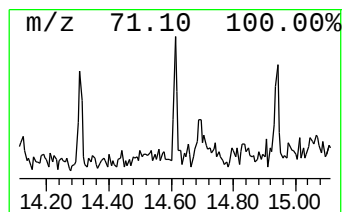
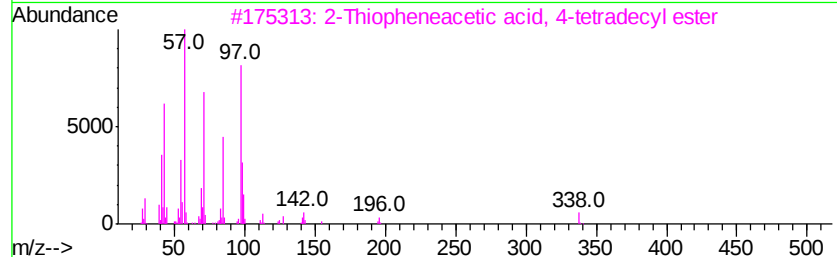
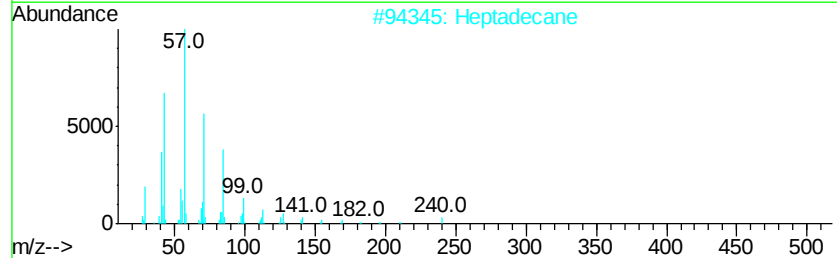
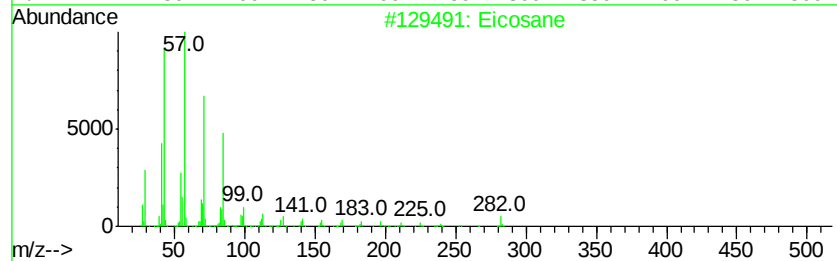
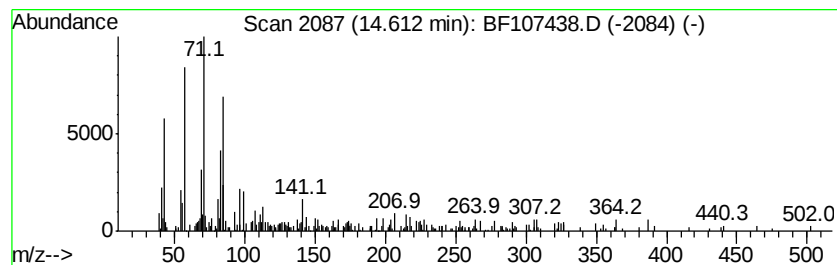
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Eicosane Concentration Rank 8

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 14.61 | 2.36 ng | 163860 | Chrysene-d12     | 14.17 |

| Hit# | of | Tentative ID                        | MW  | MolForm     | CAS#         | Qual |
|------|----|-------------------------------------|-----|-------------|--------------|------|
| 1    | 5  | Eicosane                            | 282 | C20H42      | 000112-95-8  | 58   |
| 2    |    | Heptadecane                         | 240 | C17H36      | 000629-78-7  | 52   |
| 3    |    | 2-Thiopheneacetic acid, 4-tetrad... | 338 | C20H34O2S   | 1000280-67-0 | 47   |
| 4    |    | Hexadecane                          | 226 | C16H34      | 000544-76-3  | 46   |
| 5    |    | Benzamide, N-tetrahydrofurfuryl-... | 273 | C13H14F3N02 | 1000306-93-3 | 38   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF071718\  
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Acq On : 17 Jul 2018 10:12  
Operator : JU/SJ  
Sample : J3633-01  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

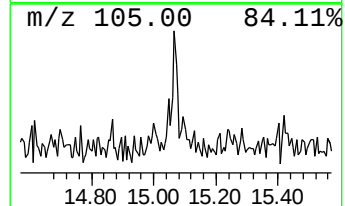
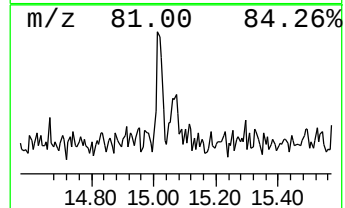
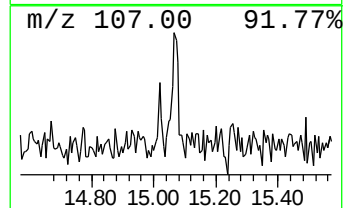
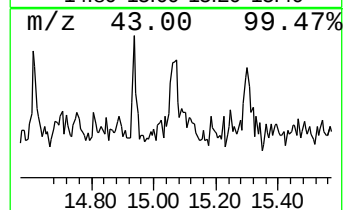
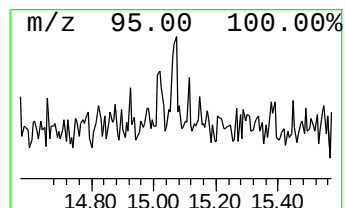
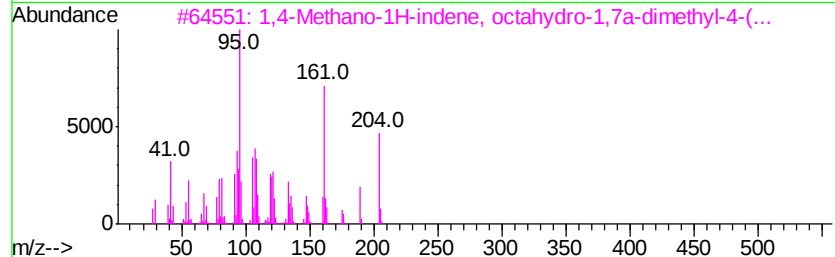
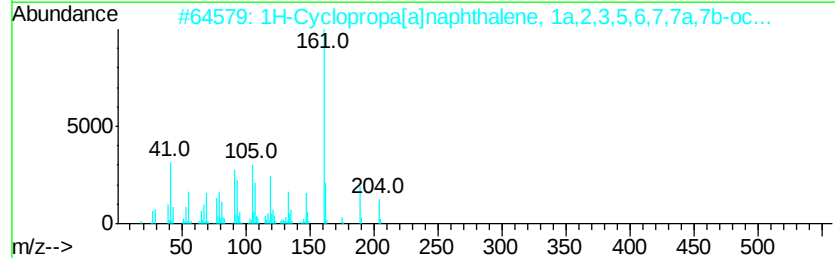
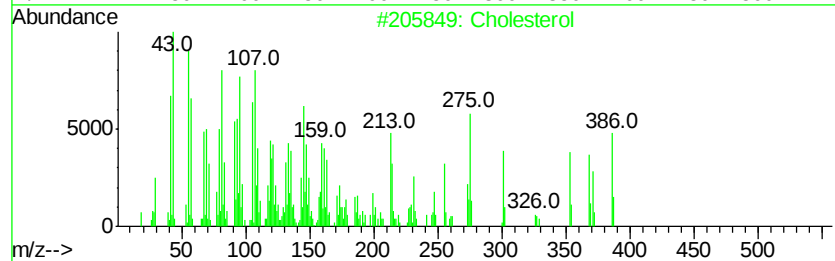
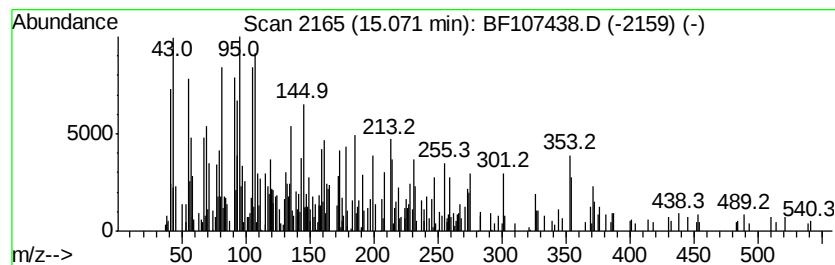
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 unknown15.07 Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 15.07 | 6.86 ng | 433600 | Perylene-d12     | 15.70 |

| Hit# | of | Tentative ID                        | MW  | MolForm | CAS#         | Qual |
|------|----|-------------------------------------|-----|---------|--------------|------|
| 1    | 5  | Cholesterol                         | 386 | C27H46O | 000057-88-5  | 49   |
| 2    |    | 1H-Cyclopropa[a]naphthalene, 1a,... | 204 | C15H24  | 017334-55-3  | 46   |
| 3    |    | 1,4-Methano-1H-indene, octahydro... | 204 | C15H24  | 087064-18-4  | 46   |
| 4    |    | Azulene, 1,2,3,5,6,7,8,8a-octahy... | 204 | C15H24  | 003691-11-0  | 30   |
| 5    |    | Cycloheptane, 4-methylene-1-meth... | 204 | C15H24  | 1000159-38-5 | 30   |



Data Path : Z:\SVOASRV\HPCHEM1\BNA\_F\DATA\BF071718\  
Data File : BF107438.D  
Acq On : 17 Jul 2018 10:12  
Operator : JU/SJ  
Sample : J3633-01  
Misc :  
ALS Vial : 3 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
A-1(0-6)

Quant Method : Z:\SVOASRV\HPCHEM1\BNA\_F\METHODS\8270-BF071618.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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-hy... | 5.22  | 8.3     | ng    | 410456   | 1                     | 6.98  | 983742  | 20.0 |
| unknown6.75          | 6.75  | 67.1    | ng    | 3298740  | 1                     | 6.98  | 983742  | 20.0 |
| Pentadecanoic acid   | 12.02 | 4.0     | ng    | 307957   | 4                     | 11.52 | 1553650 | 20.0 |
| 9-Octadecenamide,... | 12.16 | 4.8     | ng    | 368702   | 4                     | 11.52 | 1553650 | 20.0 |
| 9-Tricosene, (Z)-    | 13.98 | 5.5     | ng    | 385035   | 5                     | 14.17 | 1388250 | 20.0 |
| Eicosane             | 14.61 | 2.4     | ng    | 163860   | 5                     | 14.17 | 1388250 | 20.0 |
| unknown15.07         | 15.07 | 6.9     | ng    | 433600   | 6                     | 15.70 | 1264050 | 20.0 |