

Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
 Data File : BF103616.D  
 Acq On : 13 Mar 2018 20:36  
 Operator : SJ/JU  
 Sample : J1898-03  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF022218.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         | 5.104       | 510           | 513         | 525          | rBV2     | 29806          | 69596         | 2.08%           | 0.220%        |
| 2         | 5.487       | 575           | 578         | 621          | rBV      | 1147336        | 3156851       | 94.19%          | 9.998%        |
| 3         | 6.498       | 747           | 750         | 769          | rBV      | 1516825        | 3089621       | 92.19%          | 9.785%        |
| 4         | 6.628       | 769           | 772         | 798          | rVB      | 2252752        | 3351445       | 100.00%         | 10.614%       |
| 5         | 6.857       | 808           | 811         | 833          | rVB      | 423473         | 819065        | 24.44%          | 2.594%        |
| 6         | 7.010       | 833           | 837         | 864          | rVB      | 1864943        | 2422137       | 72.27%          | 7.671%        |
| 7         | 7.428       | 904           | 908         | 932          | rBV      | 1187848        | 2186853       | 65.25%          | 6.926%        |
| 8         | 8.139       | 1026          | 1029        | 1053         | rBV      | 586692         | 1080584       | 32.24%          | 3.422%        |
| 9         | 9.075       | 1185          | 1188        | 1196         | rVB      | 140370         | 143719        | 4.29%           | 0.455%        |
| 10        | 9.186       | 1204          | 1207        | 1208         | rBV      | 143863         | 113662        | 3.39%           | 0.360%        |
| 11        | 9.210       | 1208          | 1211        | 1226         | rVV      | 2714534        | 3198627       | 95.44%          | 10.130%       |
| 12        | 9.316       | 1226          | 1229        | 1237         | rVV2     | 45325          | 83702         | 2.50%           | 0.265%        |
| 13        | 9.416       | 1240          | 1246        | 1261         | rVV5     | 36574          | 128595        | 3.84%           | 0.407%        |
| 14        | 9.898       | 1324          | 1328        | 1342         | rBV      | 989884         | 1164983       | 34.76%          | 3.690%        |
| 15        | 10.281      | 1389          | 1393        | 1395         | rBV      | 60893          | 49889         | 1.49%           | 0.158%        |
| 16        | 10.692      | 1460          | 1463        | 1476         | rBV      | 1324016        | 1981727       | 59.13%          | 6.276%        |
| 17        | 11.227      | 1550          | 1554        | 1557         | rBV2     | 26397          | 34009         | 1.01%           | 0.108%        |
| 18        | 11.322      | 1565          | 1570        | 1574         | rBV3     | 29991          | 33528         | 1.00%           | 0.106%        |
| 19        | 11.392      | 1579          | 1582        | 1597         | rBV      | 879527         | 1257939       | 37.53%          | 3.984%        |
| 20        | 11.539      | 1603          | 1607        | 1612         | rBV      | 161521         | 156321        | 4.66%           | 0.495%        |
| 21        | 11.598      | 1613          | 1617        | 1624         | rBV5     | 28197          | 45384         | 1.35%           | 0.144%        |
| 22        | 11.657      | 1624          | 1627        | 1629         | rBV      | 41862          | 37895         | 1.13%           | 0.120%        |
| 23        | 11.904      | 1666          | 1669        | 1672         | rBV      | 189088         | 220332        | 6.57%           | 0.698%        |
| 24        | 11.933      | 1672          | 1674        | 1680         | rVB      | 913629         | 872113        | 26.02%          | 2.762%        |
| 25        | 12.063      | 1693          | 1696        | 1699         | rVB      | 50374          | 39857         | 1.19%           | 0.126%        |
| 26        | 12.451      | 1759          | 1762        | 1767         | rVB      | 75138          | 64371         | 1.92%           | 0.204%        |
| 27        | 12.774      | 1813          | 1817        | 1819         | rBV      | 64718          | 56923         | 1.70%           | 0.180%        |
| 28        | 12.827      | 1823          | 1826        | 1828         | rBV      | 116317         | 103101        | 3.08%           | 0.327%        |
| 29        | 12.974      | 1847          | 1851        | 1863         | rBV      | 2255062        | 2494700       | 74.44%          | 7.901%        |
| 30        | 13.180      | 1881          | 1886        | 1890         | rBV      | 175076         | 196683        | 5.87%           | 0.623%        |
| 31        | 13.480      | 1934          | 1937        | 1941         | rVB      | 53411          | 48068         | 1.43%           | 0.152%        |
| 32        | 13.521      | 1941          | 1944        | 1948         | rBV      | 150028         | 141280        | 4.22%           | 0.447%        |
| 33        | 13.851      | 1997          | 2000        | 2007         | rBV      | 594434         | 678150        | 20.23%          | 2.148%        |
| 34        | 13.992      | 2021          | 2024        | 2030         | rVB      | 69189          | 67377         | 2.01%           | 0.213%        |

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Misc :  
ALS Vial : 21 Sample Multiplier: 1

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:\HPCHEM1\BNA\_F\METHODS\8270-BF022218.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

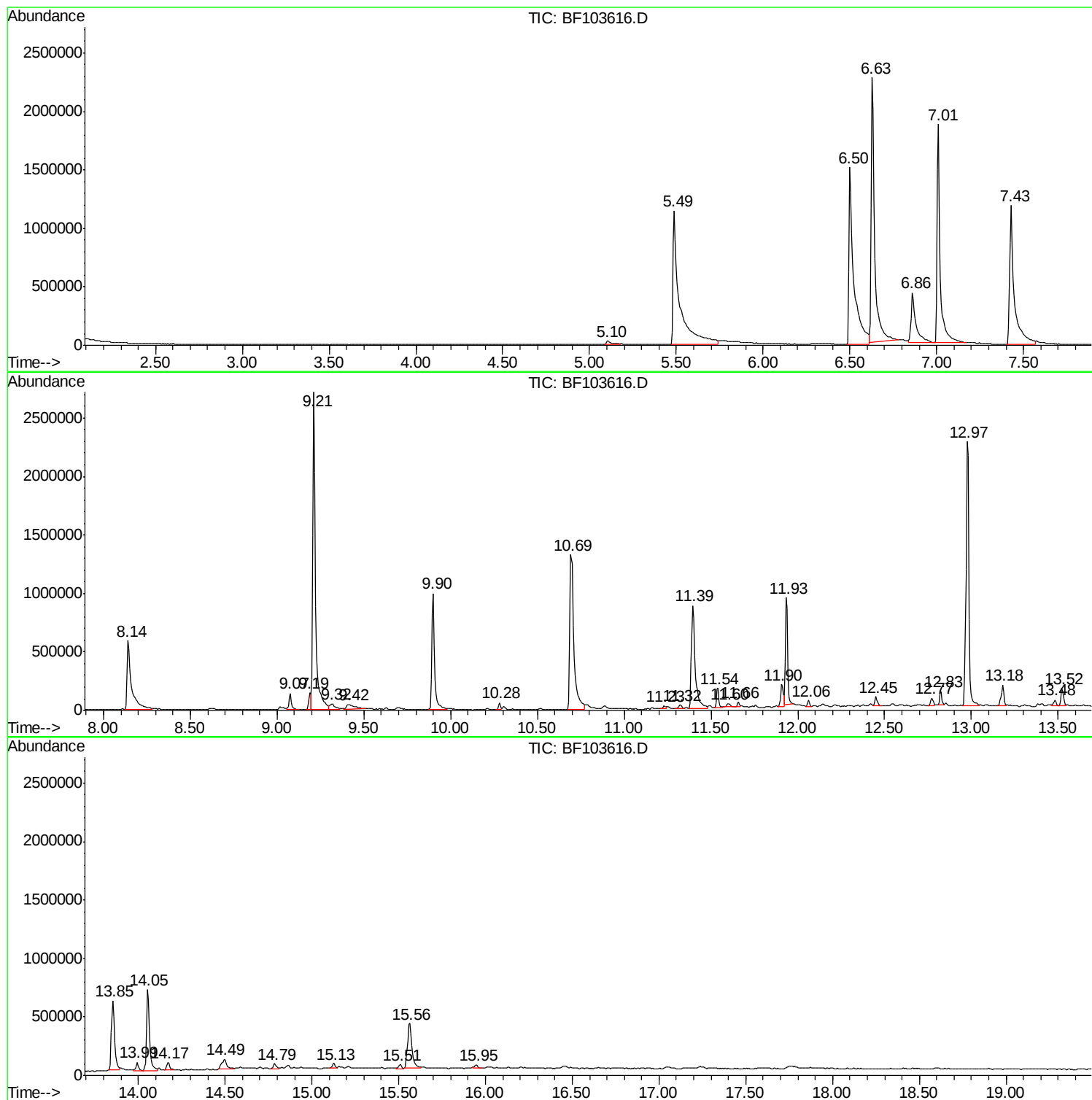
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|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 14.051 | 2030 | 2034 | 2044 | rBV  | 689837 | 870520 | 25.97% | 2.757% |
| 36 | 14.168 | 2051 | 2054 | 2060 | rBV  | 61509  | 72614  | 2.17%  | 0.230% |
| 37 | 14.492 | 2104 | 2109 | 2119 | rBV2 | 82373  | 174908 | 5.22%  | 0.554% |
| 38 | 14.786 | 2155 | 2159 | 2163 | rBV  | 45491  | 55408  | 1.65%  | 0.175% |
| 39 | 15.127 | 2213 | 2217 | 2220 | rBV  | 39436  | 47534  | 1.42%  | 0.151% |
| 40 | 15.510 | 2278 | 2282 | 2285 | rVB2 | 33239  | 43210  | 1.29%  | 0.137% |
| 41 | 15.563 | 2286 | 2291 | 2302 | rBV  | 384191 | 682583 | 20.37% | 2.162% |
| 42 | 15.951 | 2353 | 2357 | 2362 | rVB2 | 26219  | 38863  | 1.16%  | 0.123% |

Sum of corrected areas: 31574727

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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.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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Sample : J1898-03  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

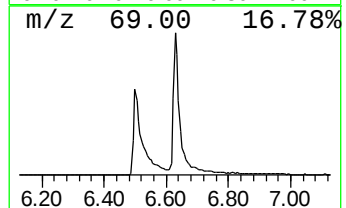
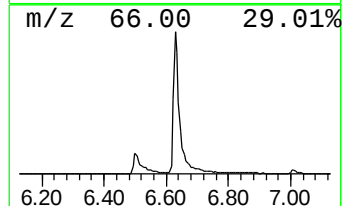
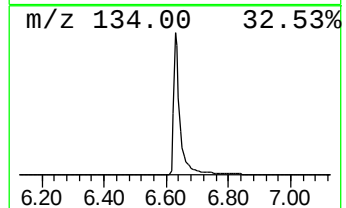
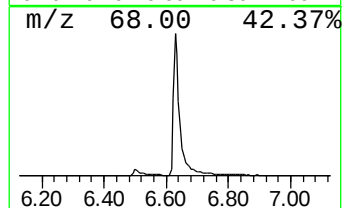
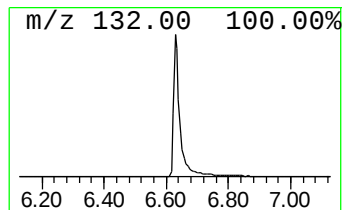
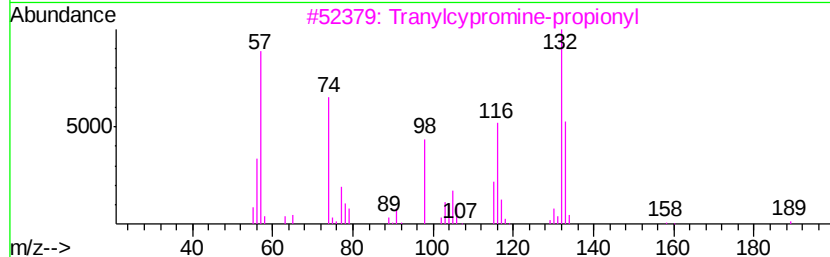
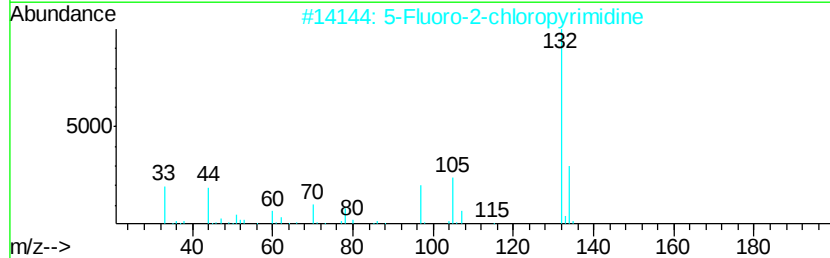
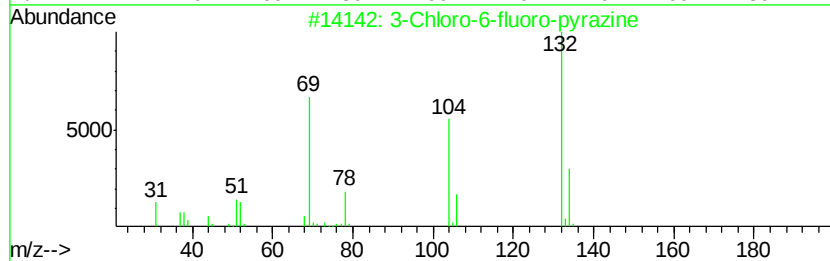
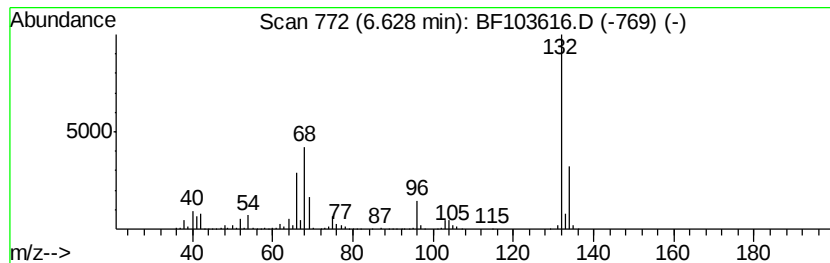
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 unknown6.63 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.63 | 81.84 ng | 3351450 | 1,4-Dichlorobenzene-d4 | 6.86 |

| Hit# | of | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|-------------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | 5-Fluoro-2-chloropyrimidine         | 132 | C4H2ClFN2 | 062802-42-0  | 16   |
| 3    |    | Tranvlcypramine-propionyl           | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 4    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 5    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4  | 9    |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

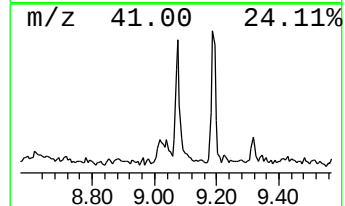
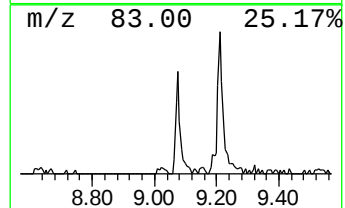
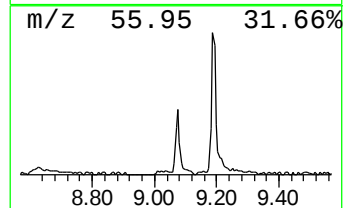
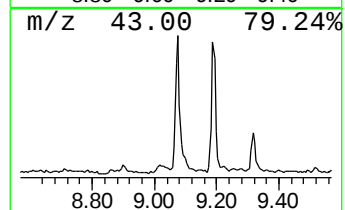
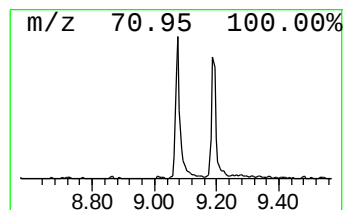
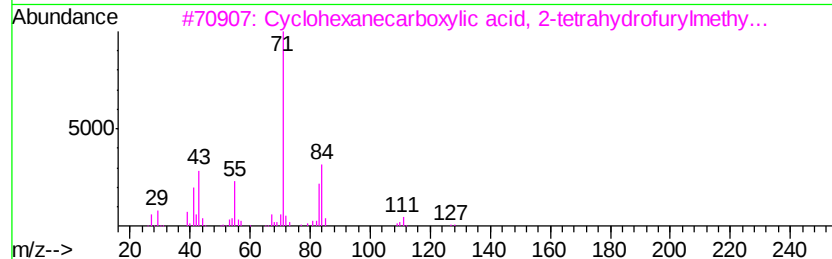
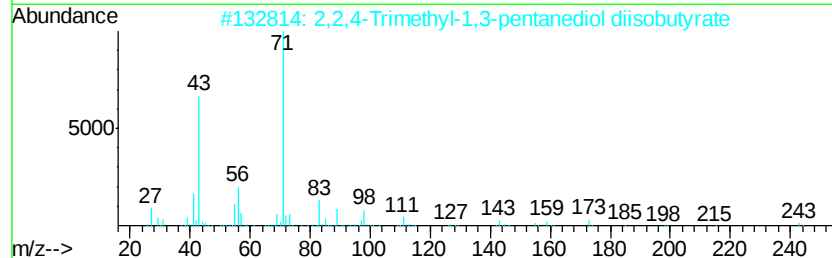
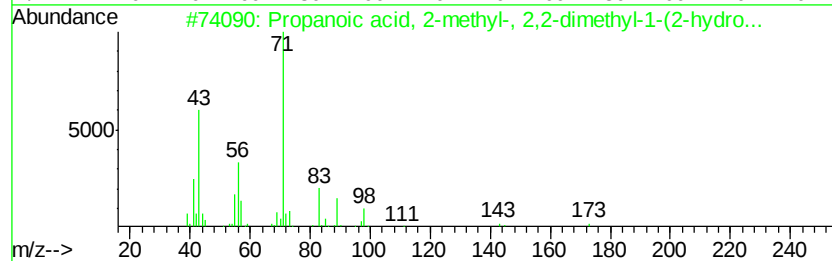
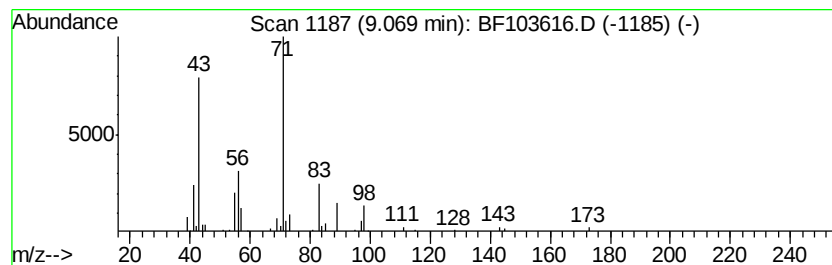
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 3 Propanoic acid, 2-methyl-, ... Concentration Rank 8

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.07 | 2.47 ng | 143719 | Acenaphthene-d10 | 9.90 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#         | Qual |
|------|----|-------------------------------------|-----|----------|--------------|------|
| 1    | 5  | Propanoic acid, 2-methyl-, 2,2-d... | 216 | C12H24O3 | 074367-33-2  | 86   |
| 2    |    | 2,2,4-Trimethyl-1,3-pentanediol ... | 286 | C16H30O4 | 006846-50-0  | 64   |
| 3    |    | Cyclohexanecarboxylic acid, 2-te... | 212 | C12H20O3 | 1000279-85-7 | 53   |
| 4    |    | Butanoic acid, 2-methylpropyl ester | 144 | C8H16O2  | 000539-90-2  | 42   |
| 5    |    | Propanoic acid, 2-methyl-, 1-(1,... | 286 | C16H30O4 | 074381-40-1  | 40   |



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Misc :  
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
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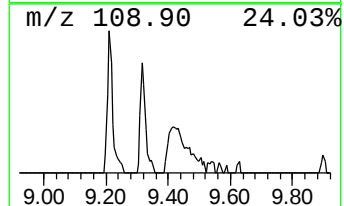
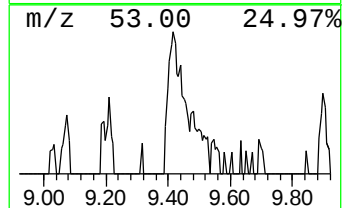
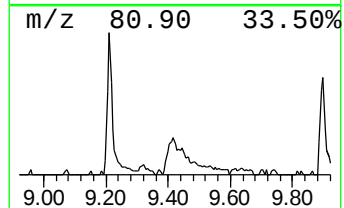
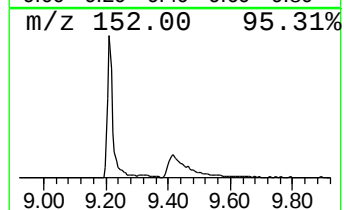
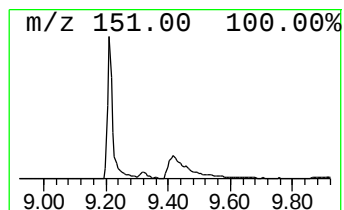
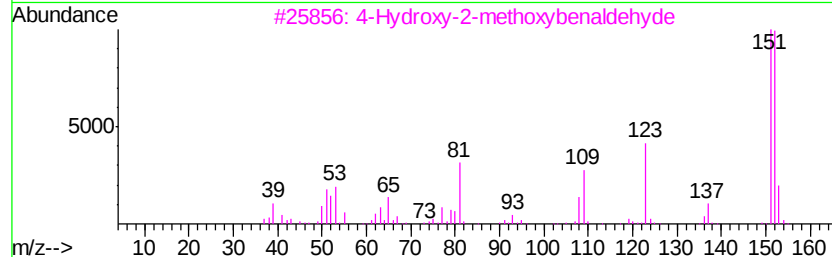
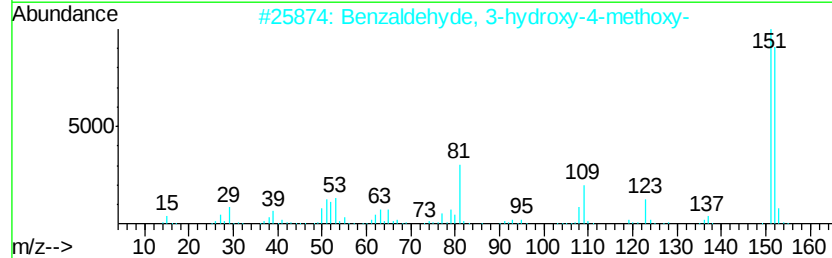
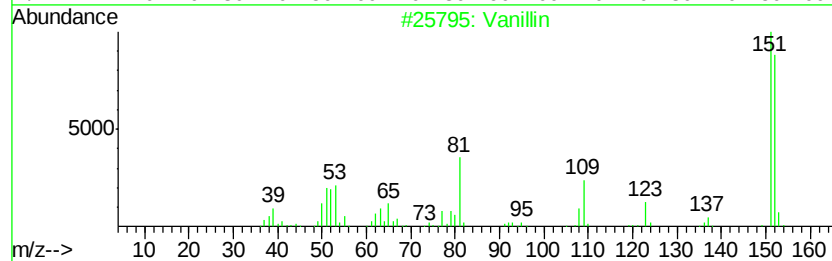
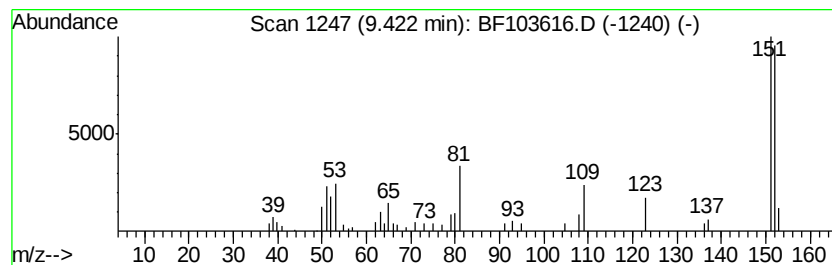
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Vanillin Concentration Rank 10

| R.T. | EstConc | Area   | Relative to ISTD | R.T. |
|------|---------|--------|------------------|------|
| 9.42 | 2.21 ng | 128595 | Acenaphthene-d10 | 9.90 |

| Hit# of | 5                                  | Tentative ID | MW  | MolForm   | CAS#         | Qual |
|---------|------------------------------------|--------------|-----|-----------|--------------|------|
| 1       | Vanillin                           |              | 152 | C8H8O3    | 000121-33-5  | 97   |
| 2       | Benzaldehyde, 3-hydroxy-4-methoxy- |              | 152 | C8H8O3    | 000621-59-0  | 93   |
| 3       | 4-Hydroxy-2-methoxybenzaldehyde    |              | 152 | C8H8O3    | 018278-34-7  | 72   |
| 4       | Vanillin lactoside                 |              | 476 | C20H28O13 | 1000129-94-7 | 64   |
| 5       | Benzaldehyde, 2-hydroxy-4-methoxy- |              | 152 | C8H8O3    | 000673-22-3  | 59   |



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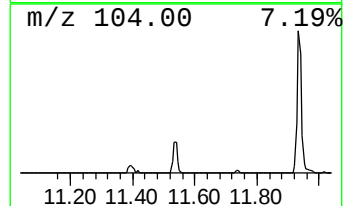
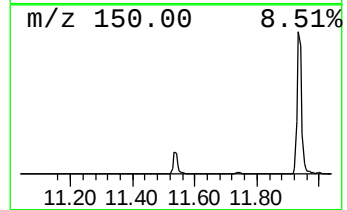
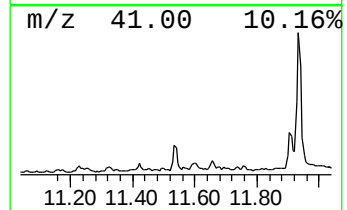
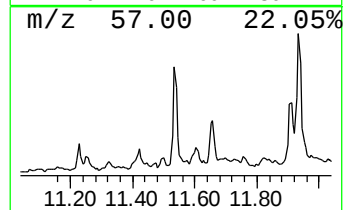
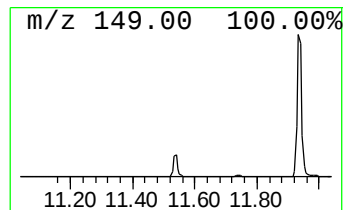
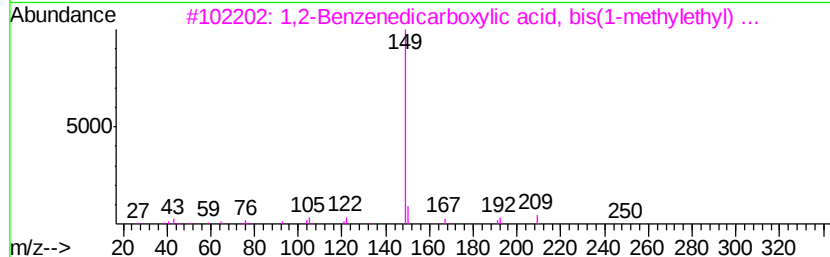
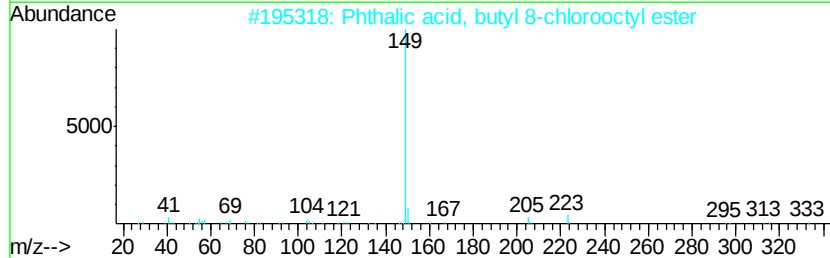
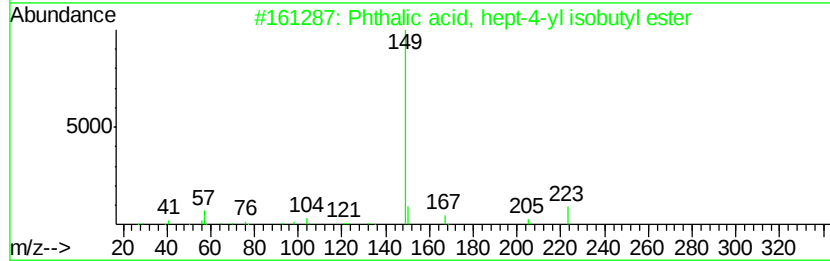
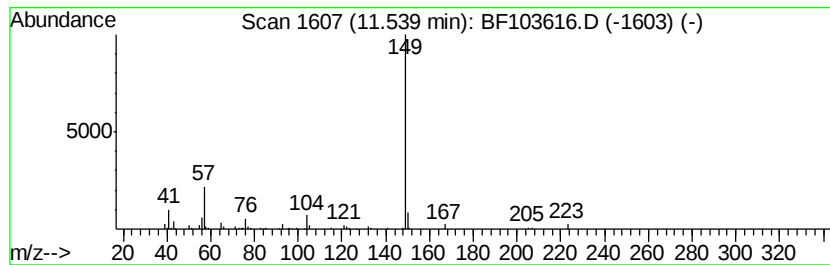
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 Phthalic acid, hept-4-yl is... Concentration Rank 7

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 11.54 | 2.49 ng | 156321 | Phenanthrene-d10 | 11.39 |

| Hit# of | 5 | Tentative ID                         | MW  | MolForm    | CAS#         | Qual |
|---------|---|--------------------------------------|-----|------------|--------------|------|
| 1       |   | Phthalic acid, hept-4-yl isobutyl... | 320 | C19H28O4   | 1000356-78-3 | 83   |
| 2       |   | Phthalic acid, butyl 8-chlorooct...  | 368 | C20H29ClO4 | 1000356-85-9 | 83   |
| 3       |   | 1,2-Benzenedicarboxylic acid, bi...  | 250 | C14H18O4   | 000605-45-8  | 78   |
| 4       |   | Phthalic acid, 2,4-dimethylpent...   | 320 | C19H28O4   | 1000356-84-3 | 78   |
| 5       |   | 1,2-Benzenedicarboxylic acid, bu...  | 304 | C18H24O4   | 000084-64-0  | 78   |



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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

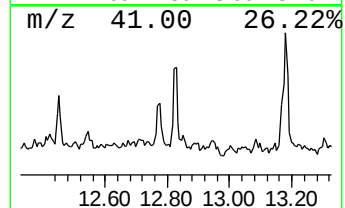
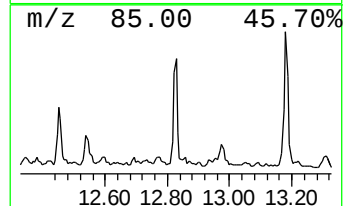
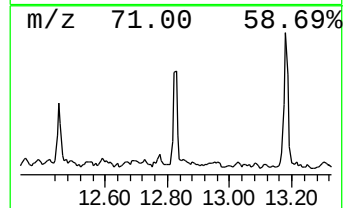
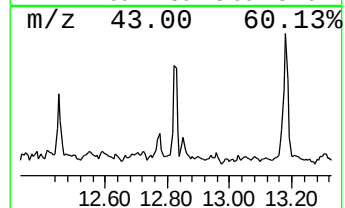
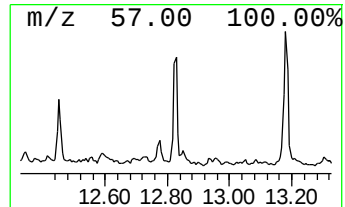
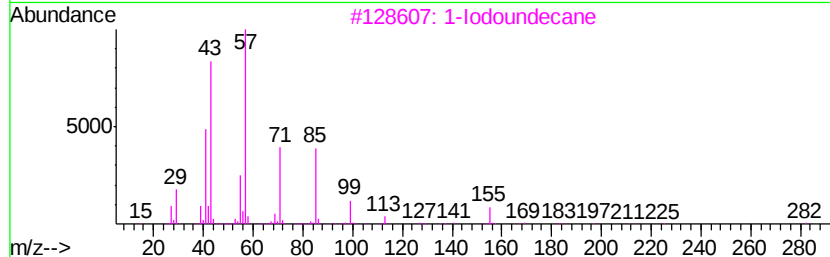
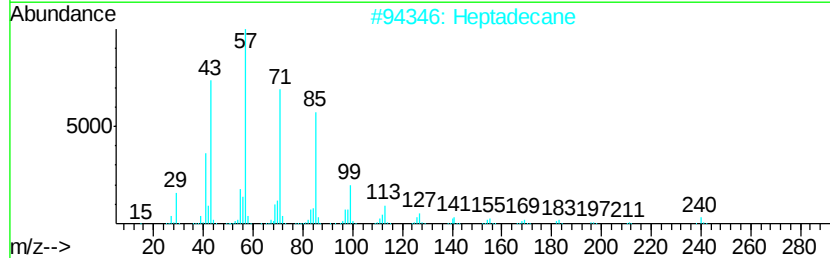
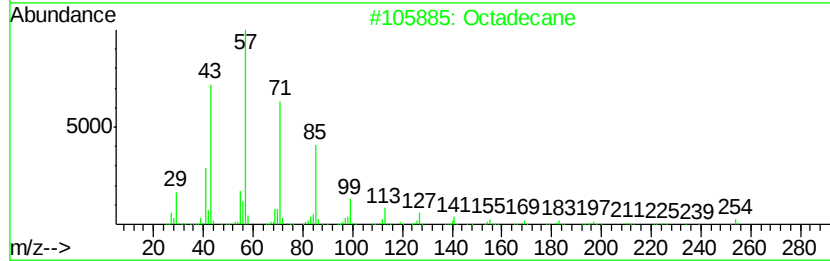
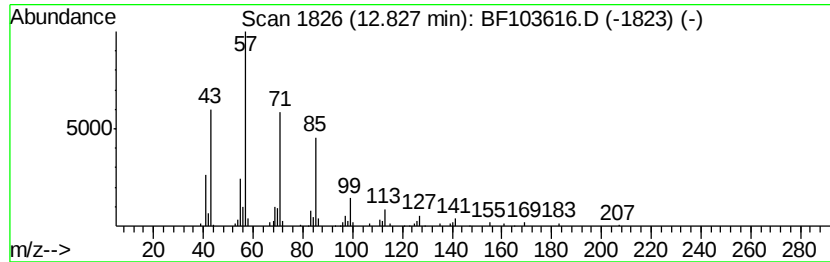
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 Octadecane Concentration Rank 9

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 12.83 | 2.37 ng | 103101 | Chrysene-d12     | 14.05 |

| Hit# | of | Tentative ID   | MW  | MolForm | CAS#        | Qual |
|------|----|----------------|-----|---------|-------------|------|
| 1    | 5  | Octadecane     | 254 | C18H38  | 000593-45-3 | 86   |
| 2    |    | Heptadecane    | 240 | C17H36  | 000629-78-7 | 86   |
| 3    |    | 1-Iodoundecane | 282 | C11H23I | 004282-44-4 | 80   |
| 4    |    | Heptacosane    | 380 | C27H56  | 000593-49-7 | 74   |
| 5    |    | Tetracosane    | 338 | C24H50  | 000646-31-1 | 74   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
Data File : BF103616.D  
Acq On : 13 Mar 2018 20:36  
Operator : SJ/JU  
Sample : J1898-03  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

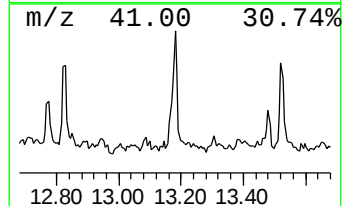
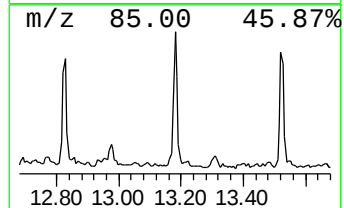
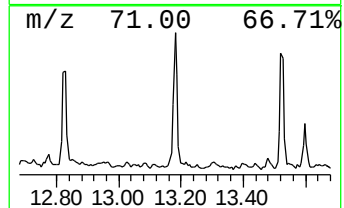
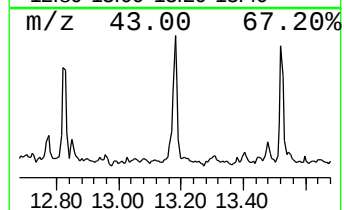
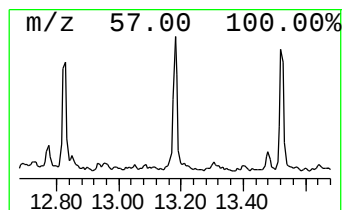
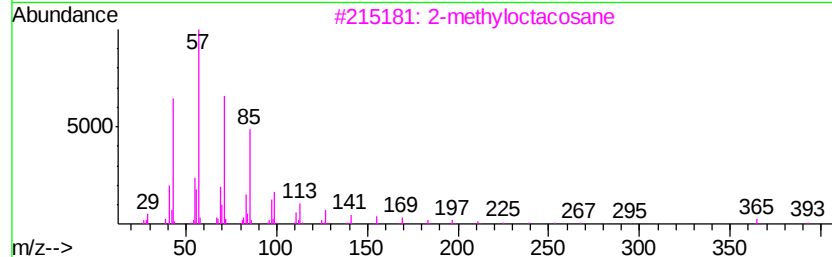
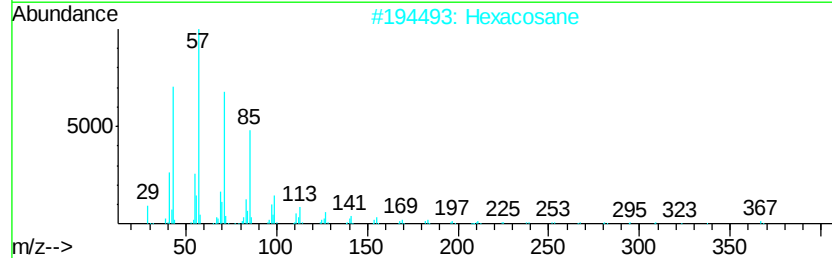
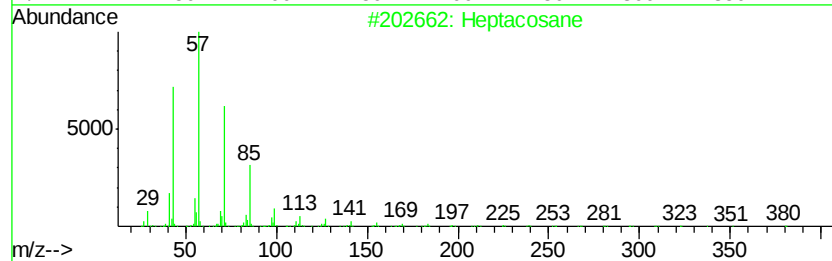
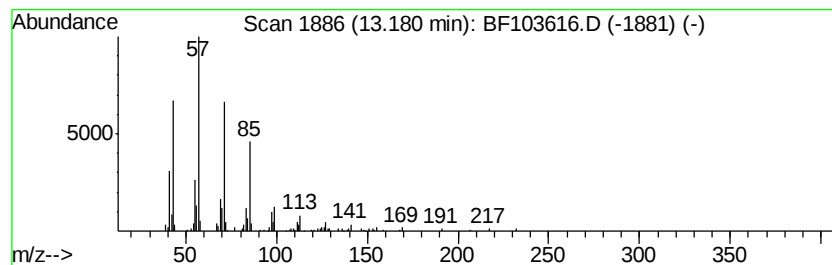
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 7 Heptacosane Concentration Rank 4

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.18 | 4.52 ng | 196683 | Chrysene-d12     | 14.05 |

| Hit# | of | Tentative ID       | MW  | MolForm | CAS#         | Qual |
|------|----|--------------------|-----|---------|--------------|------|
| 1    | 5  | Heptacosane        | 380 | C27H56  | 000593-49-7  | 91   |
| 2    |    | Hexacosane         | 366 | C26H54  | 000630-01-3  | 91   |
| 3    |    | 2-methyloctacosane | 408 | C29H60  | 1000376-72-8 | 91   |
| 4    |    | Heneicosane        | 296 | C21H44  | 000629-94-7  | 91   |
| 5    |    | Tetratetracontane  | 619 | C44H90  | 007098-22-8  | 91   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
Data File : BF103616.D  
Acq On : 13 Mar 2018 20:36  
Operator : SJ/JU  
Sample : J1898-03  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

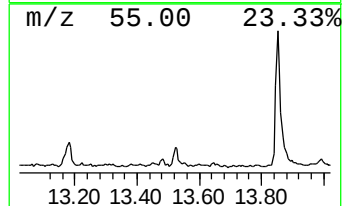
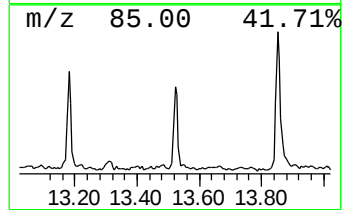
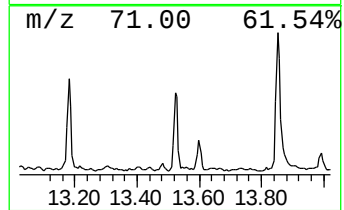
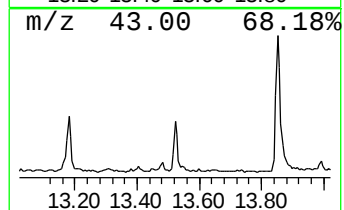
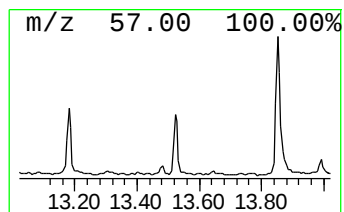
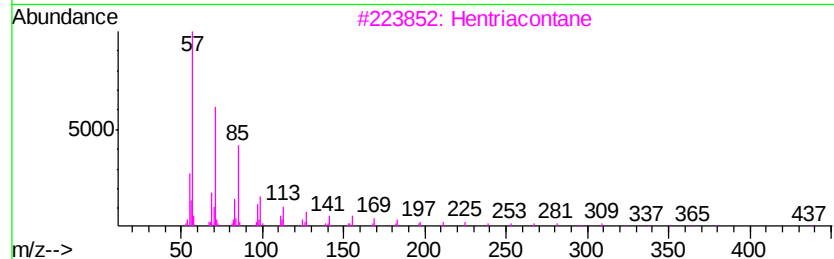
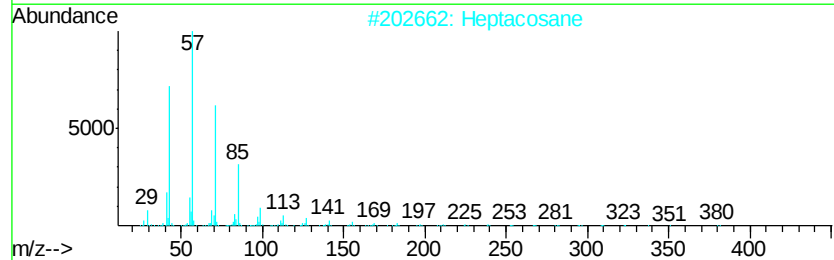
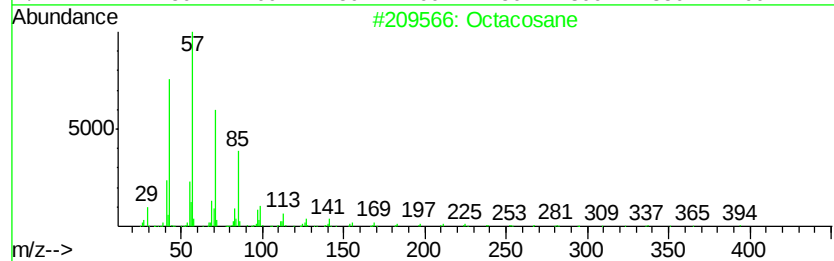
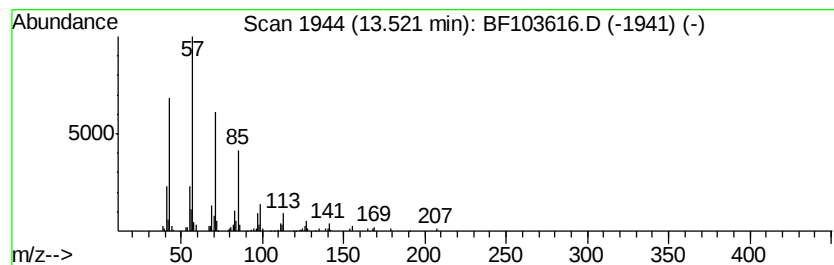
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 8 Octacosane Concentration Rank 6

| R.T.  | EstConc | Area   | Relative to ISTD | R.T.  |
|-------|---------|--------|------------------|-------|
| 13.52 | 3.25 ng | 141280 | Chrysene-d12     | 14.05 |

| Hit# | of | Tentative ID      | MW  | MolForm | CAS#        | Qual |
|------|----|-------------------|-----|---------|-------------|------|
| 1    | 5  | Octacosane        | 394 | C28H58  | 000630-02-4 | 91   |
| 2    |    | Heptacosane       | 380 | C27H56  | 000593-49-7 | 91   |
| 3    |    | Hentriacontane    | 437 | C31H64  | 000630-04-6 | 91   |
| 4    |    | Tetratetracontane | 619 | C44H90  | 007098-22-8 | 91   |
| 5    |    | Hexatriacontane   | 507 | C36H74  | 000630-06-8 | 91   |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF031318\  
Data File : BF103616.D  
Acq On : 13 Mar 2018 20:36  
Operator : SJ/JU  
Sample : J1898-03  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF022218.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

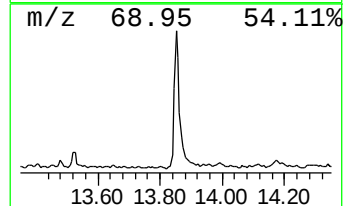
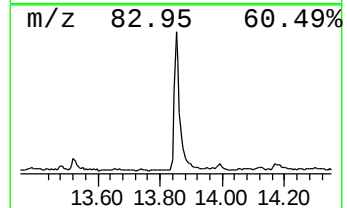
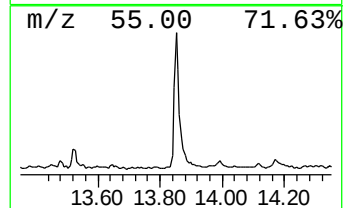
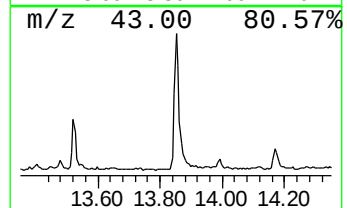
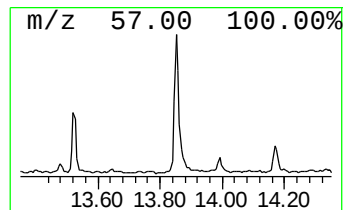
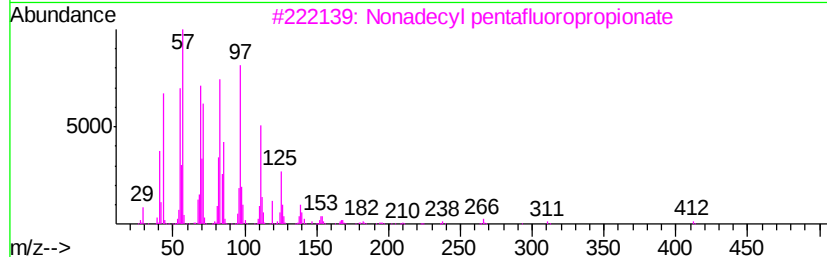
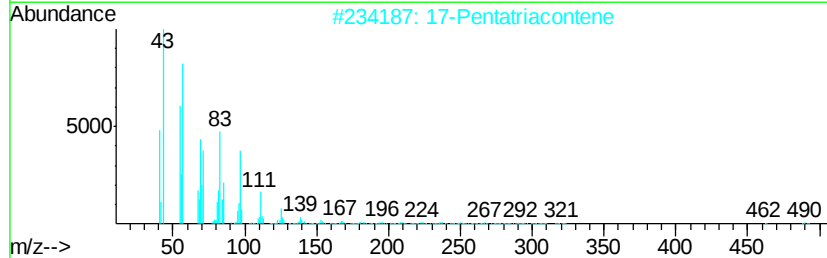
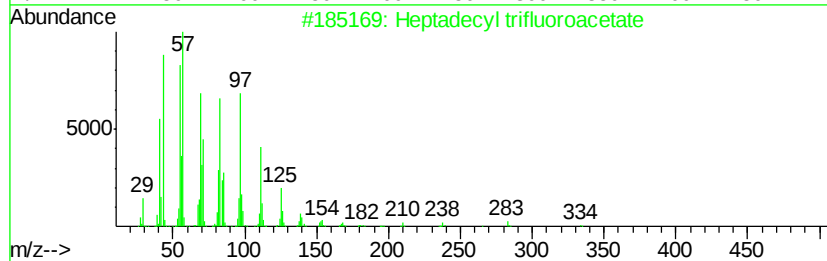
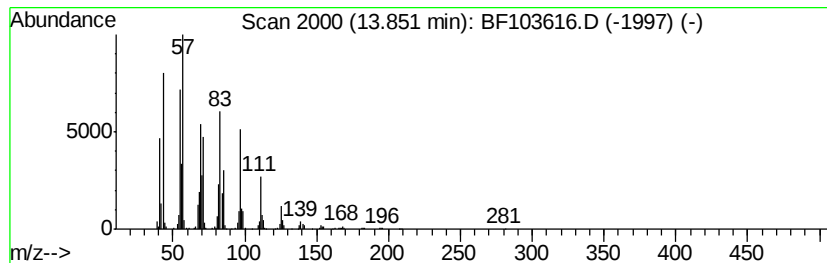
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 9 Heptadecyl trifluoroacetate Concentration Rank 3

| R.T.  | EstConc  | Area   | Relative to ISTD | R.T.  |
|-------|----------|--------|------------------|-------|
| 13.85 | 15.58 ng | 678150 | Chrysene-d12     | 14.05 |

| Hit# | of | Tentative ID                    | MW  | MolForm    | CAS#         | Qual |
|------|----|---------------------------------|-----|------------|--------------|------|
| 1    | 5  | Heptadecyl trifluoroacetate     | 352 | C19H35F3O2 | 1000351-87-0 | 91   |
| 2    |    | 17-Pentatriacontene             | 491 | C35H70     | 006971-40-0  | 91   |
| 3    |    | Nonadecyl pentafluoropropionate | 430 | C22H39F5O2 | 1000351-88-8 | 91   |
| 4    |    | Octadecyl trifluoroacetate      | 366 | C20H37F3O2 | 079392-43-1  | 91   |
| 5    |    | Docosyl pentafluoropropionate   | 472 | C25H45F5O2 | 1000351-80-9 | 91   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF031318\  
Data File : BF103616.D  
Acq On : 13 Mar 2018 20:36  
Operator : SJ/JU  
Sample : J1898-03  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF022218.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 |
| unknown6.63          | 6.63  | 81.8    | ng    | 3351450  | 1                     | 6.86  | 819065  | 20.0 |
| Propanoic acid, 2... | 9.07  | 2.5     | ng    | 143719   | 3                     | 9.90  | 1164980 | 20.0 |
| Vanillin             | 9.42  | 2.2     | ng    | 128595   | 3                     | 9.90  | 1164980 | 20.0 |
| Phthalic acid, he... | 11.54 | 2.5     | ng    | 156321   | 4                     | 11.39 | 1257940 | 20.0 |
| Octadecane           | 12.83 | 2.4     | ng    | 103101   | 5                     | 14.05 | 870520  | 20.0 |
| Heptacosane          | 13.18 | 4.5     | ng    | 196683   | 5                     | 14.05 | 870520  | 20.0 |
| Octacosane           | 13.52 | 3.3     | ng    | 141280   | 5                     | 14.05 | 870520  | 20.0 |
| Heptadecyl triflu... | 13.85 | 15.6    | ng    | 678150   | 5                     | 14.05 | 870520  | 20.0 |