

Data Path : Z:\HPCHEM1\BNA F\DATA\BF062917\  
 Data File : BF096315.D  
 Acq On : 30 Jun 2017 2:06  
 Operator : SJ/MA  
 Sample : I3882-14  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 G54-1.5-3

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-BF062717.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         | 3.781       | 284           | 288         | 292          | rBV4     | 8870           | 13504         | 1.14%           | 0.091%        |
| 2         | 4.322       | 376           | 380         | 389          | rVB      | 291316         | 343509        | 28.90%          | 2.316%        |
| 3         | 4.957       | 484           | 488         | 498          | rVB      | 788768         | 785250        | 66.07%          | 5.295%        |
| 4         | 5.380       | 556           | 560         | 563          | rVB      | 870135         | 825387        | 69.44%          | 5.566%        |
| 5         | 6.392       | 728           | 732         | 741          | rVB      | 1286241        | 1188577       | 100.00%         | 8.015%        |
| 6         | 6.533       | 753           | 756         | 760          | rBV      | 1064610        | 998525        | 84.01%          | 6.734%        |
| 7         | 6.769       | 793           | 796         | 800          | rBV      | 941242         | 869778        | 73.18%          | 5.865%        |
| 8         | 6.833       | 804           | 807         | 813          | rBV      | 15455          | 16907         | 1.42%           | 0.114%        |
| 9         | 6.927       | 819           | 823         | 826          | rBV      | 1113367        | 893489        | 75.17%          | 6.025%        |
| 10        | 7.327       | 886           | 891         | 894          | rBV      | 762318         | 698911        | 58.80%          | 4.713%        |
| 11        | 7.380       | 897           | 900         | 903          | rVV2     | 15698          | 14636         | 1.23%           | 0.099%        |
| 12        | 7.416       | 903           | 906         | 912          | rVB3     | 14773          | 15316         | 1.29%           | 0.103%        |
| 13        | 8.051       | 1010          | 1014        | 1017         | rBV      | 1234127        | 1084105       | 91.21%          | 7.311%        |
| 14        | 8.486       | 1085          | 1088        | 1093         | rVB      | 14094          | 14437         | 1.21%           | 0.097%        |
| 15        | 8.657       | 1114          | 1117        | 1119         | rBV      | 21196          | 19565         | 1.65%           | 0.132%        |
| 16        | 8.686       | 1119          | 1122        | 1124         | rVB2     | 29787          | 24951         | 2.10%           | 0.168%        |
| 17        | 8.763       | 1132          | 1135        | 1140         | rVB      | 28665          | 27701         | 2.33%           | 0.187%        |
| 18        | 8.863       | 1150          | 1152        | 1156         | rBV      | 17489          | 14787         | 1.24%           | 0.100%        |
| 19        | 9.127       | 1193          | 1197        | 1200         | rBV      | 1390039        | 1090370       | 91.74%          | 7.353%        |
| 20        | 9.221       | 1209          | 1213        | 1217         | rBV2     | 25547          | 27728         | 2.33%           | 0.187%        |
| 21        | 9.398       | 1238          | 1243        | 1249         | rBV6     | 8808           | 17407         | 1.46%           | 0.117%        |
| 22        | 9.468       | 1251          | 1255        | 1257         | rBV2     | 16814          | 17035         | 1.43%           | 0.115%        |
| 23        | 9.521       | 1261          | 1264        | 1266         | rBV      | 181843         | 149836        | 12.61%          | 1.010%        |
| 24        | 9.663       | 1285          | 1288        | 1291         | rVB      | 20346          | 15846         | 1.33%           | 0.107%        |
| 25        | 9.751       | 1300          | 1303        | 1305         | rVB      | 29942          | 21448         | 1.80%           | 0.145%        |
| 26        | 9.804       | 1307          | 1312        | 1316         | rBV      | 1020581        | 889302        | 74.82%          | 5.997%        |
| 27        | 10.010      | 1344          | 1347        | 1350         | rVB      | 27780          | 22017         | 1.85%           | 0.148%        |
| 28        | 10.086      | 1355          | 1360        | 1365         | rBV      | 15551          | 26168         | 2.20%           | 0.176%        |
| 29        | 10.251      | 1384          | 1388        | 1391         | rVB      | 30163          | 27475         | 2.31%           | 0.185%        |
| 30        | 10.351      | 1403          | 1405        | 1407         | rBV2     | 20132          | 14828         | 1.25%           | 0.100%        |
| 31        | 10.468      | 1420          | 1425        | 1430         | rBV3     | 16479          | 22551         | 1.90%           | 0.152%        |
| 32        | 10.586      | 1441          | 1445        | 1449         | rBV      | 207053         | 166916        | 14.04%          | 1.126%        |
| 33        | 10.721      | 1464          | 1468        | 1469         | rBV      | 43450          | 36042         | 3.03%           | 0.243%        |
| 34        | 10.733      | 1469          | 1470        | 1474         | rVB      | 30016          | 24951         | 2.10%           | 0.168%        |

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G54-1.5-3

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-BF062717.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |        |        |        |
|----|--------|------|------|------|------|---------|--------|--------|--------|
| 35 | 11.086 | 1528 | 1530 | 1536 | rVB6 | 13179   | 18403  | 1.55%  | 0.124% |
| 36 | 11.139 | 1536 | 1539 | 1542 | rBV5 | 10963   | 15195  | 1.28%  | 0.102% |
| 37 | 11.168 | 1542 | 1544 | 1547 | rVV2 | 32718   | 33449  | 2.81%  | 0.226% |
| 38 | 11.198 | 1547 | 1549 | 1553 | rVB4 | 17098   | 16312  | 1.37%  | 0.110% |
| 39 | 11.245 | 1553 | 1557 | 1560 | rBV3 | 10408   | 14589  | 1.23%  | 0.098% |
| 40 | 11.286 | 1560 | 1564 | 1566 | rVV  | 946410  | 776372 | 65.32% | 5.235% |
| 41 | 11.310 | 1566 | 1568 | 1571 | rVV  | 129639  | 101743 | 8.56%  | 0.686% |
| 42 | 11.357 | 1573 | 1576 | 1580 | rVB  | 57952   | 52845  | 4.45%  | 0.356% |
| 43 | 11.515 | 1600 | 1603 | 1606 | rBV2 | 15770   | 19405  | 1.63%  | 0.131% |
| 44 | 11.592 | 1613 | 1616 | 1619 | rBV2 | 21047   | 24716  | 2.08%  | 0.167% |
| 45 | 11.786 | 1646 | 1649 | 1651 | rBV2 | 22919   | 18622  | 1.57%  | 0.126% |
| 46 | 11.815 | 1651 | 1654 | 1659 | rVB2 | 62128   | 52974  | 4.46%  | 0.357% |
| 47 | 11.898 | 1664 | 1668 | 1670 | rBV3 | 35190   | 41124  | 3.46%  | 0.277% |
| 48 | 11.998 | 1683 | 1685 | 1688 | rBV3 | 14825   | 13976  | 1.18%  | 0.094% |
| 49 | 12.080 | 1696 | 1699 | 1701 | rBV2 | 14322   | 17196  | 1.45%  | 0.116% |
| 50 | 12.339 | 1740 | 1743 | 1747 | rBV4 | 26136   | 27029  | 2.27%  | 0.182% |
| 51 | 12.386 | 1749 | 1751 | 1754 | rVV3 | 22573   | 21280  | 1.79%  | 0.144% |
| 52 | 12.415 | 1754 | 1756 | 1761 | rVV6 | 11652   | 17855  | 1.50%  | 0.120% |
| 53 | 12.492 | 1766 | 1769 | 1773 | rVV  | 208332  | 178652 | 15.03% | 1.205% |
| 54 | 12.721 | 1802 | 1808 | 1811 | rBV  | 200605  | 236049 | 19.86% | 1.592% |
| 55 | 12.868 | 1829 | 1833 | 1839 | rVB  | 1054958 | 893363 | 75.16% | 6.024% |
| 56 | 13.115 | 1873 | 1875 | 1878 | rVB2 | 37049   | 29990  | 2.52%  | 0.202% |
| 57 | 13.568 | 1950 | 1952 | 1955 | rVB3 | 61517   | 56793  | 4.78%  | 0.383% |
| 58 | 13.774 | 1984 | 1987 | 1993 | rVB3 | 100549  | 138081 | 11.62% | 0.931% |
| 59 | 13.915 | 2007 | 2011 | 2014 | rBV  | 948217  | 975262 | 82.05% | 6.577% |
| 60 | 14.221 | 2061 | 2063 | 2067 | rVB4 | 79646   | 65211  | 5.49%  | 0.440% |
| 61 | 14.674 | 2138 | 2140 | 2143 | rBV  | 89132   | 79782  | 6.71%  | 0.538% |
| 62 | 15.345 | 2250 | 2254 | 2258 | rVB  | 402203  | 473531 | 39.84% | 3.193% |

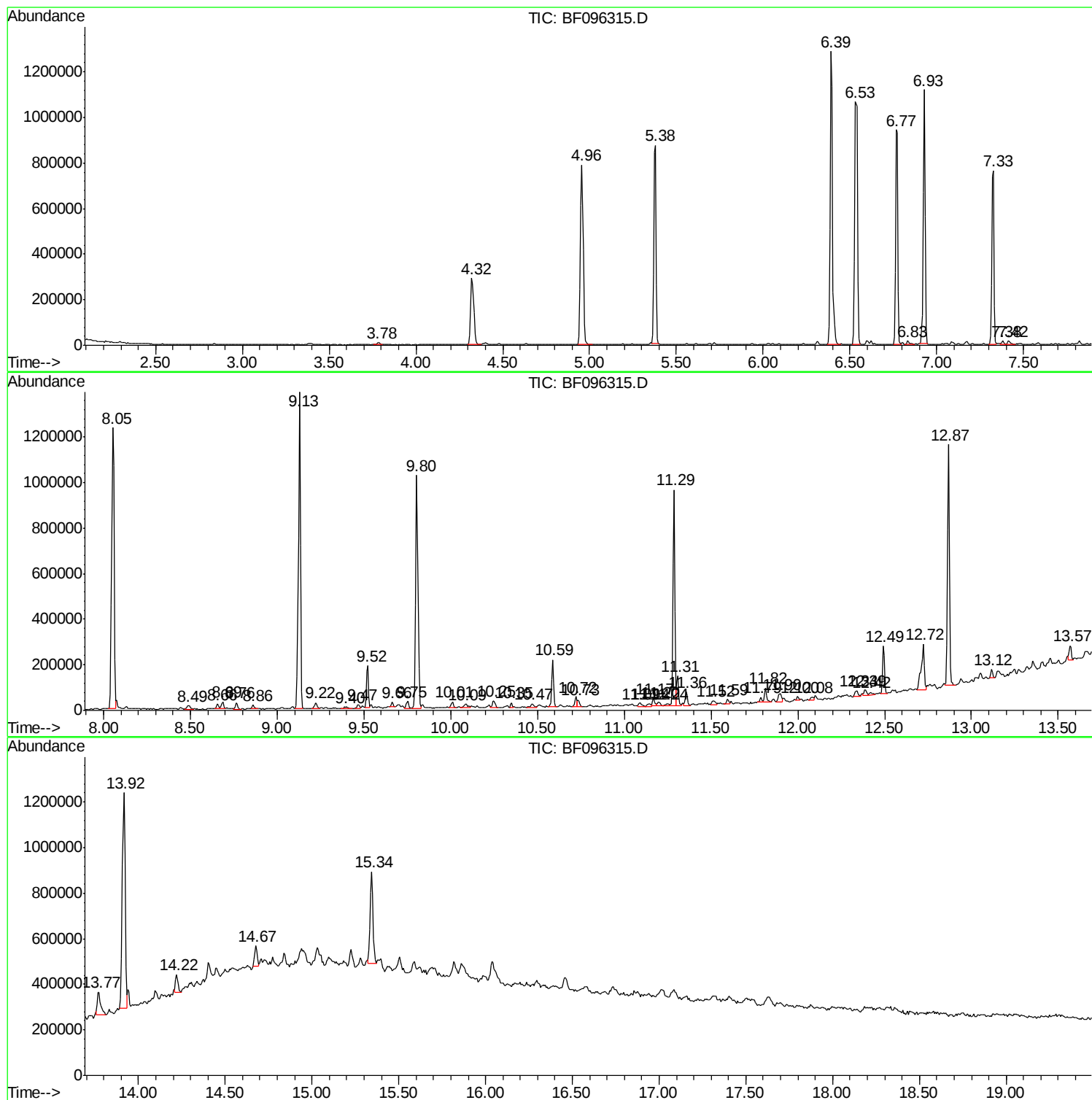
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Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampled :  
G54-1.5-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.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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Misc :  
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Instrument :  
BNA\_F  
ClientSampleId :  
G54-1.5-3

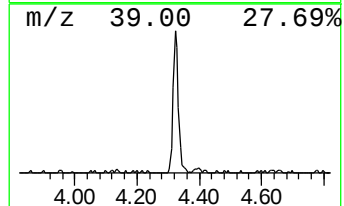
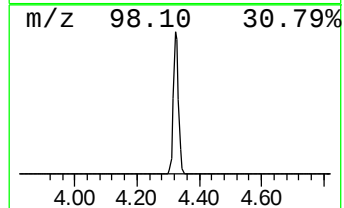
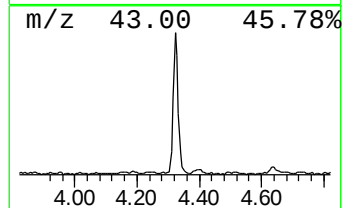
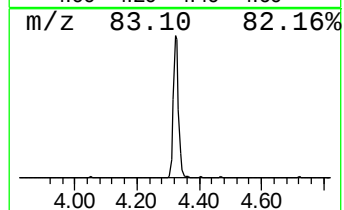
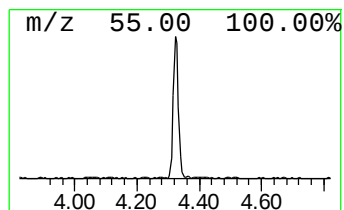
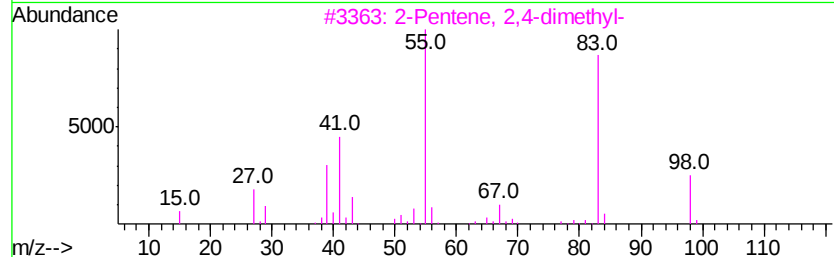
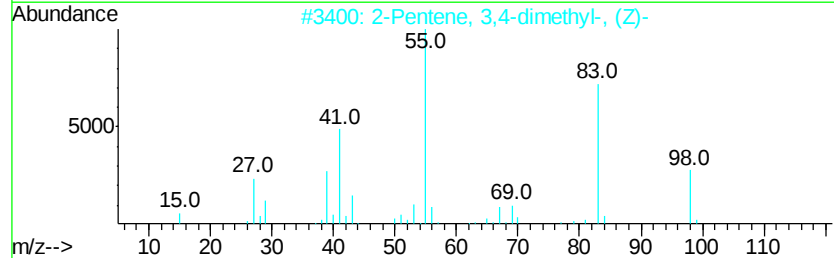
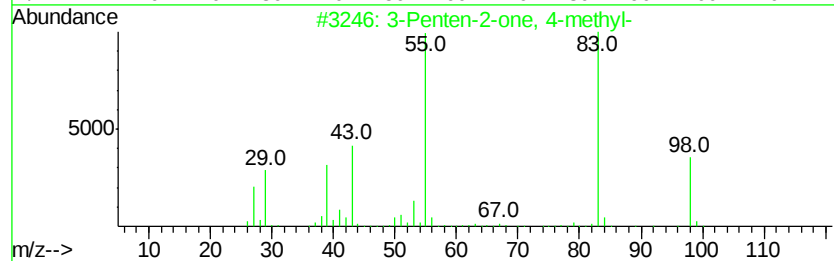
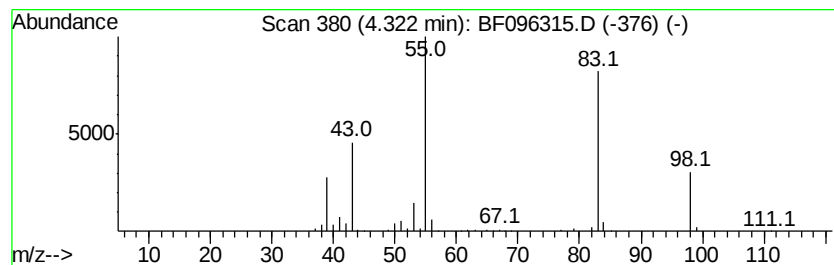
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 4

| R.T. | EstConc | Area   | Relative to ISTD       | R.T. |
|------|---------|--------|------------------------|------|
| 4.32 | 7.90 ng | 343509 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | 5 | Tentative ID                   | MW | MolForm | CAS#        | Qual |
|------|----|---|--------------------------------|----|---------|-------------|------|
| 1    |    |   | 3-Penten-2-one, 4-methyl-      | 98 | C6H10O  | 000141-79-7 | 91   |
| 2    |    |   | 2-Pentene, 3,4-dimethyl-, (Z)- | 98 | C7H14   | 004914-91-4 | 86   |
| 3    |    |   | 2-Pentene, 2,4-dimethyl-       | 98 | C7H14   | 000625-65-0 | 86   |
| 4    |    |   | 3-Hexen-2-one                  | 98 | C6H10O  | 000763-93-9 | 80   |
| 5    |    |   | 2-Pentene, 3,4-dimethyl-, (E)- | 98 | C7H14   | 004914-92-5 | 80   |



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ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
G54-1.5-3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

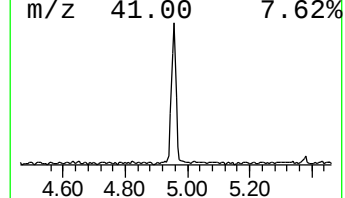
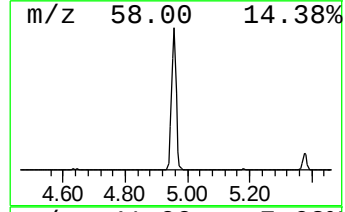
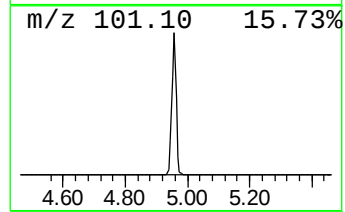
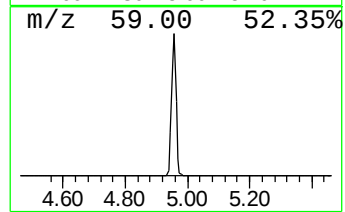
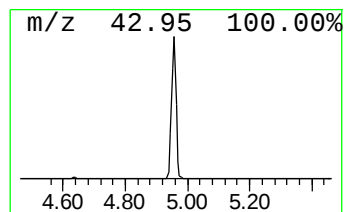
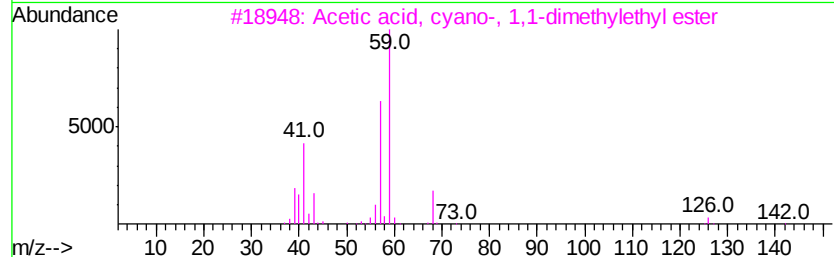
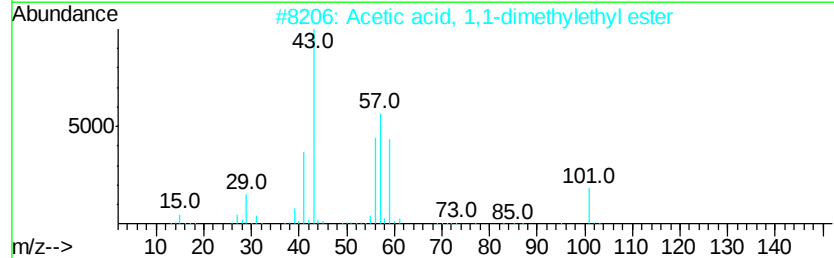
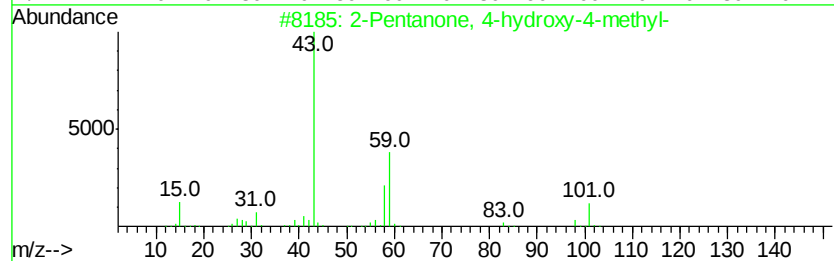
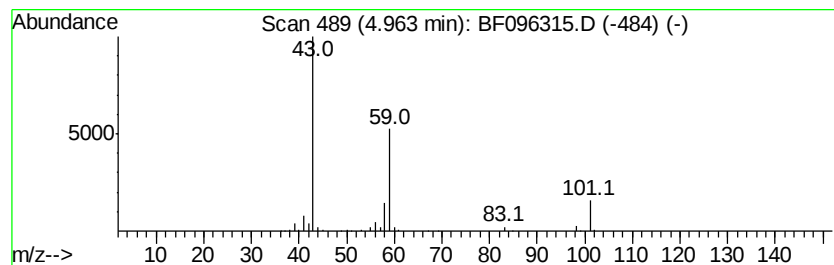
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 4.96 | 18.06 ng | 785250 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|-------------------------------------|-----|----------|-------------|------|
| 1    | 5  | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 53   |
| 2    |    | Acetic acid, 1,1-dimethylethyl e... | 116 | C6H12O2  | 000540-88-5 | 38   |
| 3    |    | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    | 2,3-Butanedione, monooxime          | 101 | C4H7NO2  | 000057-71-6 | 9    |
| 5    |    | 1-Propen-2-ol, acetate              | 100 | C5H8O2   | 000108-22-5 | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

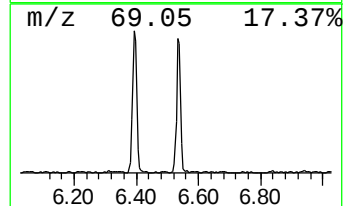
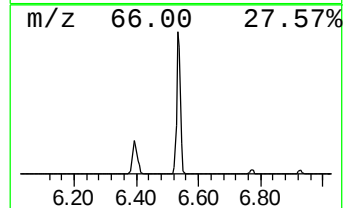
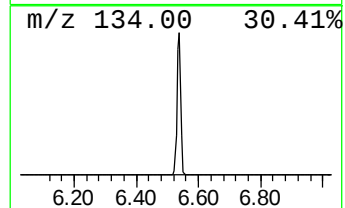
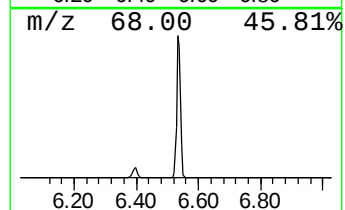
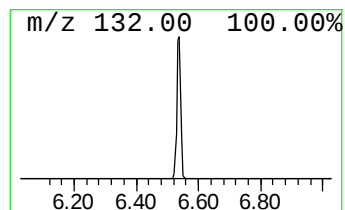
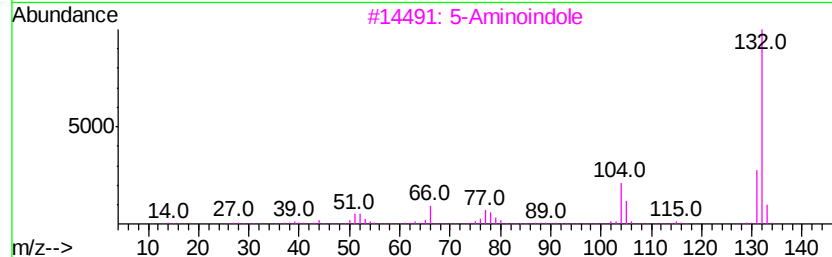
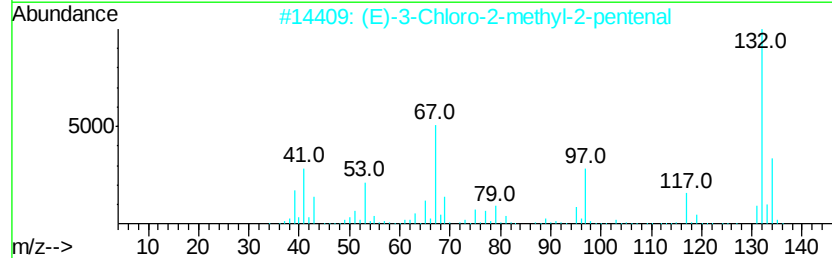
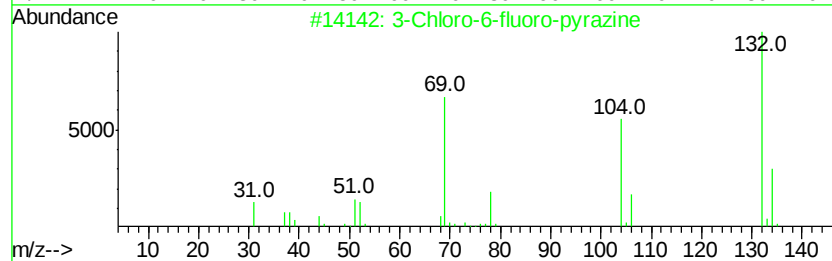
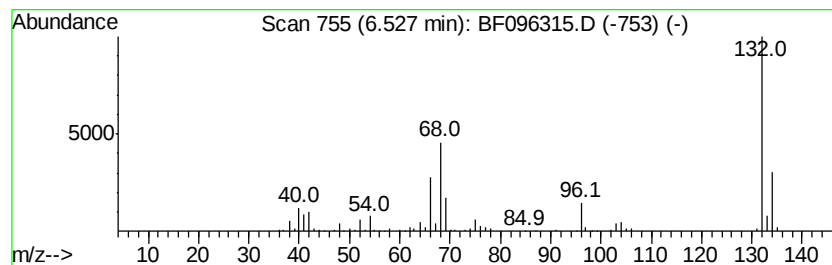
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 3 unknown6.53 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.53 | 22.96 ng | 998525 | 1,4-Dichlorobenzene-d4 | 6.77 |

| Hit# | of | Tentative ID                     | MW  | MolForm   | CAS#         | Qual |
|------|----|----------------------------------|-----|-----------|--------------|------|
| 1    | 5  | 3-Chloro-6-fluoro-pyrazine       | 132 | C4H2ClFN2 | 1000146-10-7 | 27   |
| 2    |    | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    | 5-Aminoindole                    | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    | Tranylcypromine-propionyl        | 189 | C12H15NO  | 1000123-86-3 | 10   |
| 5    |    | Amphetaminil                     | 250 | C17H18N2  | 017590-01-1  | 10   |



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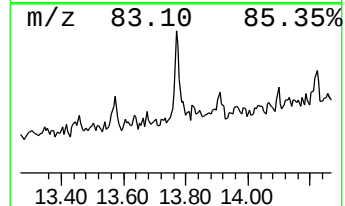
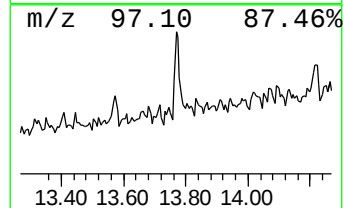
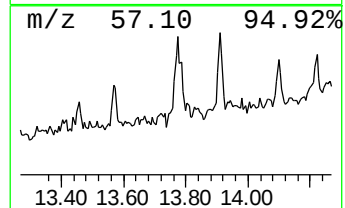
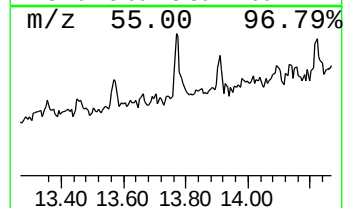
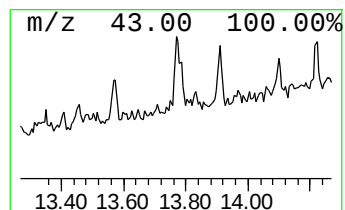
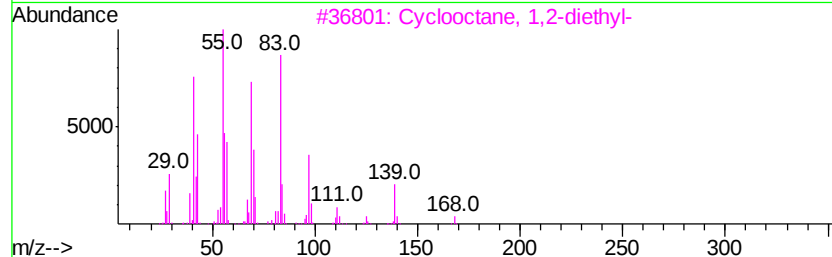
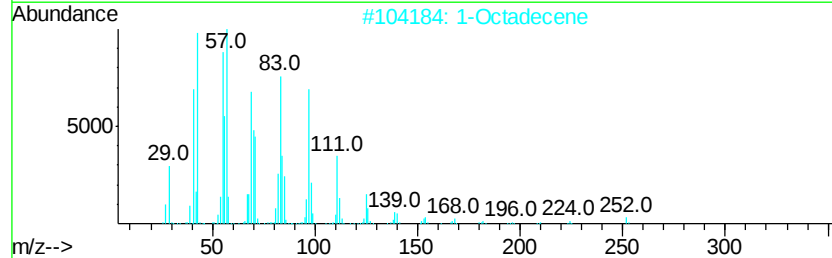
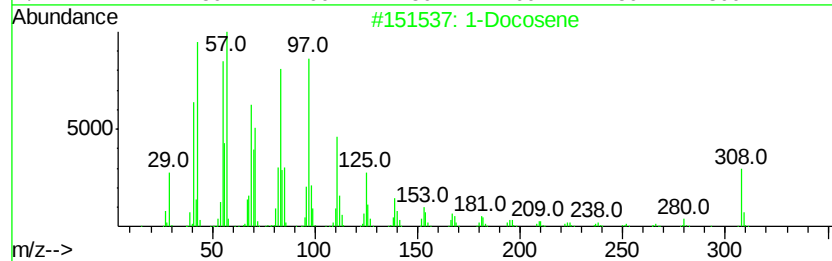
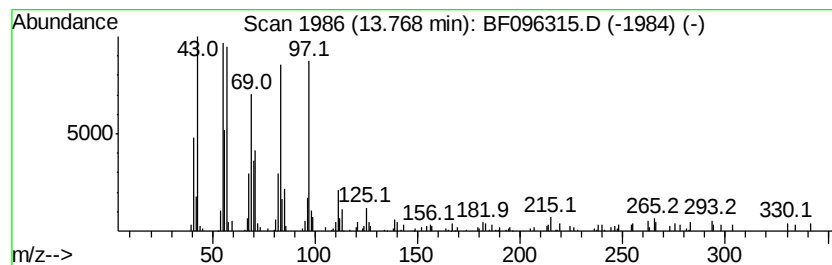
Instrument :  
BNA\_F  
ClientSampled :  
G54-1.5-3

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 5 1-Docosene Concentration Rank 6

| R.T.    | EstConc | Area                      | Relative to ISTD |         | R.T.        |      |
|---------|---------|---------------------------|------------------|---------|-------------|------|
| 13.77   | 2.83 ng | 138081                    | Chrysene-d12     |         | 13.92       |      |
| Hit# of | 5       | Tentative ID              | MW               | MolForm | CAS#        | Qual |
| 1       |         | 1-Docosene                | 308              | C22H44  | 001599-67-3 | 91   |
| 2       |         | 1-Octadecene              | 252              | C18H36  | 000112-88-9 | 62   |
| 3       |         | Cyclooctane, 1,2-diethyl- | 168              | C12H24  | 023609-46-3 | 60   |
| 4       |         | 17-Pentatriacontene       | 491              | C35H70  | 006971-40-0 | 58   |
| 5       |         | Cyclotetracosane          | 336              | C24H48  | 000297-03-0 | 55   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF062917\  
Data File : BF096315.D  
Acq On : 30 Jun 2017 2:06  
Operator : SJ/MA  
Sample : I3882-14  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
G54-1.5-3

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

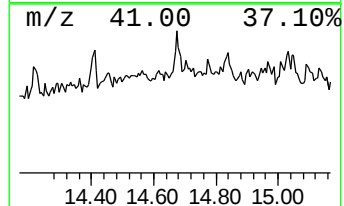
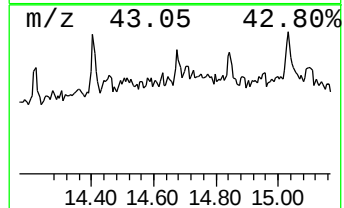
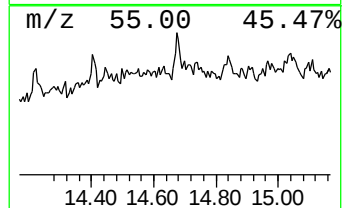
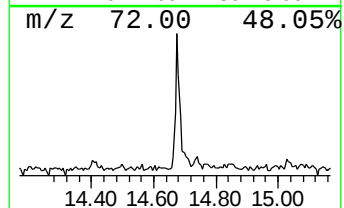
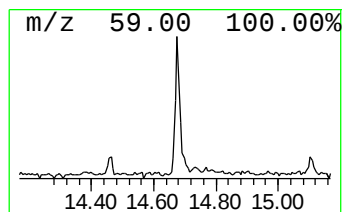
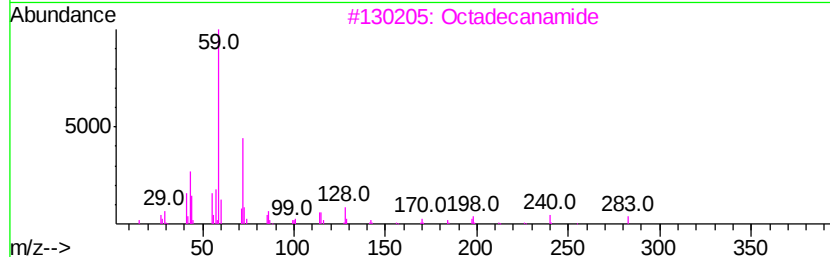
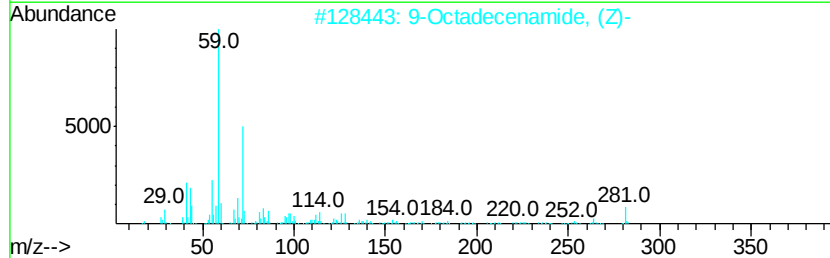
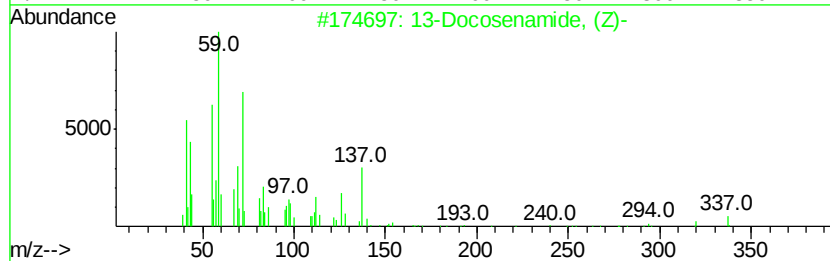
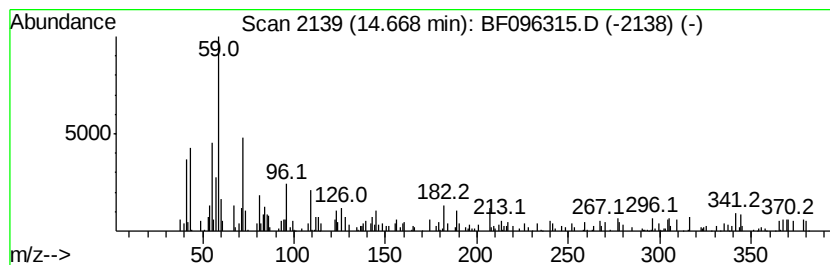
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

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Peak Number 6 13-Docosenamide, (Z)- Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 14.67 | 3.37 ng | 79782 | Perylene-d12     | 15.34 |

| Hit# | of | Tentative ID                        | MW  | MolForm    | CAS#        | Qual |
|------|----|-------------------------------------|-----|------------|-------------|------|
| 1    | 5  | 13-Docosenamide, (Z)-               | 337 | C22H43NO   | 000112-84-5 | 74   |
| 2    |    | 9-Octadecenamide, (Z)-              | 281 | C18H35NO   | 000301-02-0 | 68   |
| 3    |    | Octadecanamide                      | 283 | C18H37NO   | 000124-26-5 | 60   |
| 4    |    | Dodecanamide                        | 199 | C12H25NO   | 001120-16-7 | 49   |
| 5    |    | Benzeneethanamine, 2-fluoro-.bet... | 229 | C11H16FN03 | 061338-98-5 | 47   |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF062917\  
Data File : BF096315.D  
Acq On : 30 Jun 2017 2:06  
Operator : SJ/MA  
Sample : I3882-14  
Misc :  
ALS Vial : 21 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
G54-1.5-3

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF062717.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 |
| 3-Penten-2-one, 4... | 4.32  | 7.9     | ng    | 343509   | 1                     | 6.77  | 869778 | 20.0 |
| 2-Pentanone, 4-hy... | 4.96  | 18.1    | ng    | 785250   | 1                     | 6.77  | 869778 | 20.0 |
| unknown6.53          | 6.53  | 23.0    | ng    | 998525   | 1                     | 6.77  | 869778 | 20.0 |
| 1-Docosene           | 13.77 | 2.8     | ng    | 138081   | 5                     | 13.92 | 975262 | 20.0 |
| 13-Docosenamide, ... | 14.67 | 3.4     | ng    | 79782    | 6                     | 15.34 | 473531 | 20.0 |