

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF080317\  
 Data File : BF097341.D  
 Acq On : 4 Aug 2017 2:40  
 Operator : SJ/JU  
 Sample : I4562-04 5X  
 Misc :  
 ALS Vial : 21 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 JC-02-080117-B

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-BF072517.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         | 3.069       | 194           | 201         | 213          | rBV      | 179720         | 358229        | 43.63%          | 4.405%        |
| 2         | 4.563       | 451           | 455         | 463          | rBV      | 24245          | 36156         | 4.40%           | 0.445%        |
| 3         | 5.039       | 533           | 536         | 550          | rBV      | 343433         | 544889        | 66.36%          | 6.701%        |
| 4         | 6.116       | 716           | 719         | 733          | rVB      | 465464         | 537163        | 65.42%          | 6.606%        |
| 5         | 6.222       | 733           | 737         | 744          | rVB      | 467275         | 476212        | 58.00%          | 5.856%        |
| 6         | 6.445       | 771           | 775         | 779          | rBV      | 695261         | 583282        | 71.04%          | 7.173%        |
| 7         | 6.598       | 798           | 801         | 812          | rVB      | 352279         | 359520        | 43.79%          | 4.421%        |
| 8         | 6.810       | 834           | 837         | 840          | rBV3     | 7477           | 11131         | 1.36%           | 0.137%        |
| 9         | 7.016       | 869           | 872         | 879          | rBV      | 263843         | 246019        | 29.96%          | 3.025%        |
| 10        | 7.110       | 886           | 888         | 892          | rVB3     | 14459          | 13733         | 1.67%           | 0.169%        |
| 11        | 7.175       | 896           | 899         | 905          | rVB8     | 10916          | 15255         | 1.86%           | 0.188%        |
| 12        | 7.257       | 910           | 913         | 918          | rBV4     | 32016          | 35668         | 4.34%           | 0.439%        |
| 13        | 7.369       | 925           | 932         | 935          | rBV4     | 29156          | 37399         | 4.55%           | 0.460%        |
| 14        | 7.569       | 964           | 966         | 968          | rVB3     | 13421          | 9737          | 1.19%           | 0.120%        |
| 15        | 7.633       | 974           | 977         | 982          | rVB2     | 28565          | 31178         | 3.80%           | 0.383%        |
| 16        | 7.728       | 990           | 993         | 998          | rBV      | 990080         | 821076        | 100.00%         | 10.097%       |
| 17        | 7.904       | 1020          | 1023        | 1026         | rBV3     | 10412          | 11958         | 1.46%           | 0.147%        |
| 18        | 8.022       | 1041          | 1043        | 1046         | rVB3     | 20517          | 18048         | 2.20%           | 0.222%        |
| 19        | 8.063       | 1046          | 1050        | 1053         | rBV5     | 9661           | 15611         | 1.90%           | 0.192%        |
| 20        | 8.175       | 1066          | 1069        | 1076         | rVB4     | 28448          | 37882         | 4.61%           | 0.466%        |
| 21        | 8.233       | 1076          | 1079        | 1082         | rVB2     | 12487          | 10482         | 1.28%           | 0.129%        |
| 22        | 8.275       | 1082          | 1086        | 1090         | rBV5     | 11175          | 14167         | 1.73%           | 0.174%        |
| 23        | 8.333       | 1093          | 1096        | 1098         | rBV2     | 10430          | 11935         | 1.45%           | 0.147%        |
| 24        | 8.422       | 1109          | 1111        | 1117         | rVB5     | 14299          | 22727         | 2.77%           | 0.279%        |
| 25        | 8.616       | 1140          | 1144        | 1147         | rVB5     | 8283           | 12387         | 1.51%           | 0.152%        |
| 26        | 8.710       | 1157          | 1160        | 1164         | rBV5     | 10886          | 15419         | 1.88%           | 0.190%        |
| 27        | 8.769       | 1168          | 1170        | 1172         | rVV      | 17647          | 11075         | 1.35%           | 0.136%        |
| 28        | 8.804       | 1172          | 1176        | 1179         | rBV      | 591980         | 502271        | 61.17%          | 6.177%        |
| 29        | 9.204       | 1241          | 1244        | 1254         | rVB      | 58997          | 68952         | 8.40%           | 0.848%        |
| 30        | 9.427       | 1278          | 1282        | 1285         | rBV      | 14413          | 17638         | 2.15%           | 0.217%        |
| 31        | 9.469       | 1285          | 1289        | 1299         | rVB      | 847634         | 731478        | 89.09%          | 8.995%        |
| 32        | 9.922       | 1363          | 1366        | 1369         | rVB2     | 17279          | 13569         | 1.65%           | 0.167%        |
| 33        | 10.145      | 1397          | 1404        | 1410         | rBV4     | 12019          | 27697         | 3.37%           | 0.341%        |
| 34        | 10.257      | 1420          | 1423        | 1431         | rBV      | 225643         | 216684        | 26.39%          | 2.665%        |

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JC-02-080117-B

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-BF072517.M  
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |        |        |        |        |
|----|--------|------|------|------|------|--------|--------|--------|--------|
| 35 | 10.392 | 1443 | 1446 | 1454 | rVB2 | 19877  | 29315  | 3.57%  | 0.361% |
| 36 | 10.839 | 1517 | 1522 | 1524 | rBV  | 16769  | 16602  | 2.02%  | 0.204% |
| 37 | 10.939 | 1536 | 1539 | 1542 | rBV  | 695528 | 591511 | 72.04% | 7.274% |
| 38 | 10.963 | 1542 | 1543 | 1547 | rVB  | 29189  | 22716  | 2.77%  | 0.279% |
| 39 | 11.263 | 1591 | 1594 | 1598 | rVB2 | 14240  | 14005  | 1.71%  | 0.172% |
| 40 | 11.357 | 1606 | 1610 | 1614 | rVB7 | 9451   | 11004  | 1.34%  | 0.135% |
| 41 | 11.445 | 1620 | 1625 | 1627 | rBV3 | 11708  | 14947  | 1.82%  | 0.184% |
| 42 | 11.551 | 1640 | 1643 | 1645 | rBV3 | 15699  | 16548  | 2.02%  | 0.203% |
| 43 | 11.633 | 1653 | 1657 | 1659 | rBV5 | 7121   | 10043  | 1.22%  | 0.124% |
| 44 | 11.668 | 1659 | 1663 | 1667 | rVV4 | 17529  | 25197  | 3.07%  | 0.310% |
| 45 | 11.992 | 1715 | 1718 | 1720 | rBV3 | 17964  | 19556  | 2.38%  | 0.240% |
| 46 | 12.051 | 1725 | 1728 | 1730 | rVV2 | 23565  | 20390  | 2.48%  | 0.251% |
| 47 | 12.145 | 1741 | 1744 | 1748 | rBV  | 60808  | 58767  | 7.16%  | 0.723% |
| 48 | 12.286 | 1765 | 1768 | 1769 | rBV3 | 15261  | 15805  | 1.92%  | 0.194% |
| 49 | 12.368 | 1779 | 1782 | 1785 | rVB  | 52261  | 47202  | 5.75%  | 0.580% |
| 50 | 12.421 | 1788 | 1791 | 1798 | rVB3 | 20015  | 28946  | 3.53%  | 0.356% |
| 51 | 12.521 | 1804 | 1808 | 1816 | rVB  | 405305 | 369059 | 44.95% | 4.539% |
| 52 | 12.774 | 1848 | 1851 | 1854 | rVB2 | 22835  | 22596  | 2.75%  | 0.278% |
| 53 | 13.115 | 1906 | 1909 | 1911 | rBV  | 35649  | 30063  | 3.66%  | 0.370% |
| 54 | 13.445 | 1962 | 1965 | 1969 | rVB3 | 59959  | 65086  | 7.93%  | 0.800% |
| 55 | 13.562 | 1981 | 1985 | 1988 | rBV  | 515650 | 481307 | 58.62% | 5.919% |
| 56 | 14.351 | 2117 | 2119 | 2122 | rBV  | 53013  | 48274  | 5.88%  | 0.594% |
| 57 | 14.909 | 2210 | 2214 | 2217 | rBV  | 264751 | 296163 | 36.07% | 3.642% |

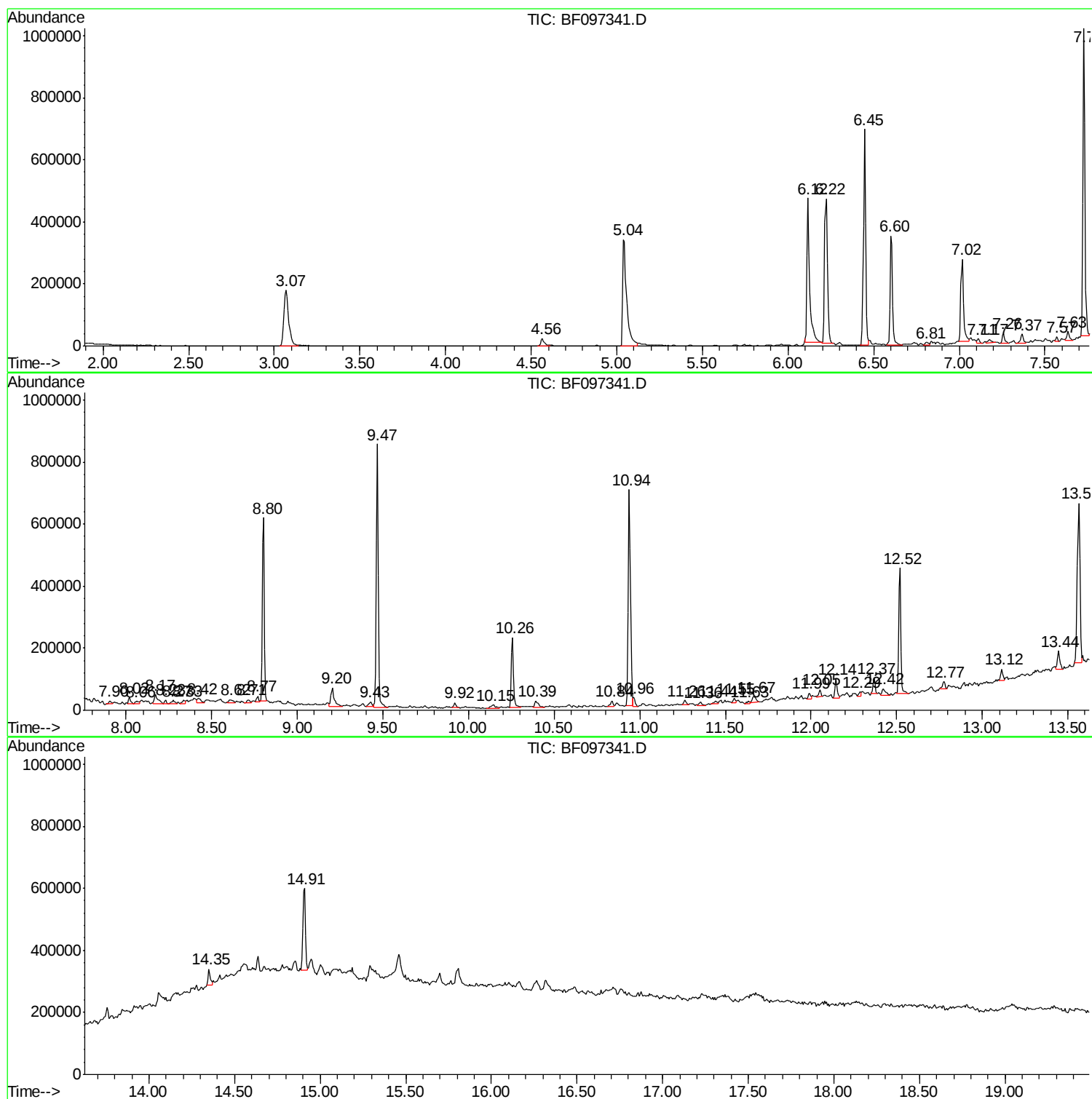
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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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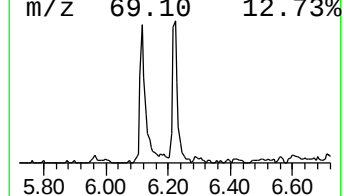
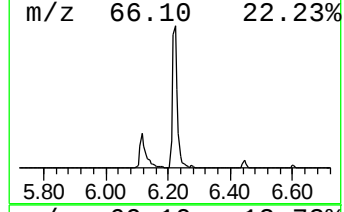
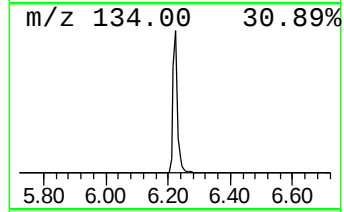
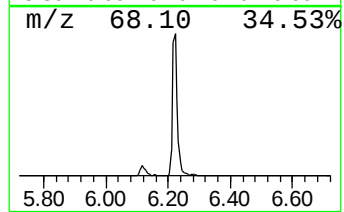
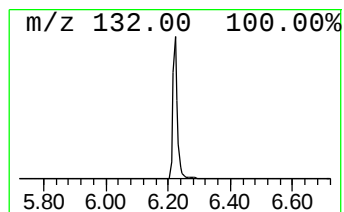
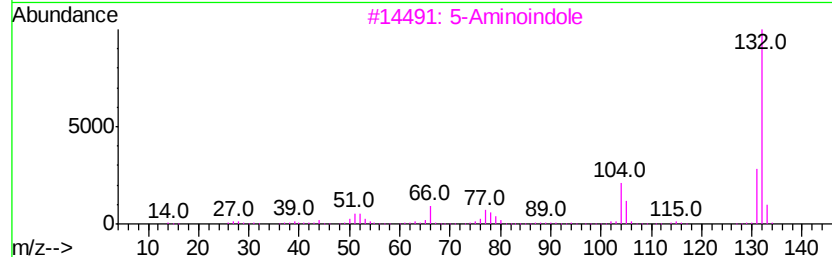
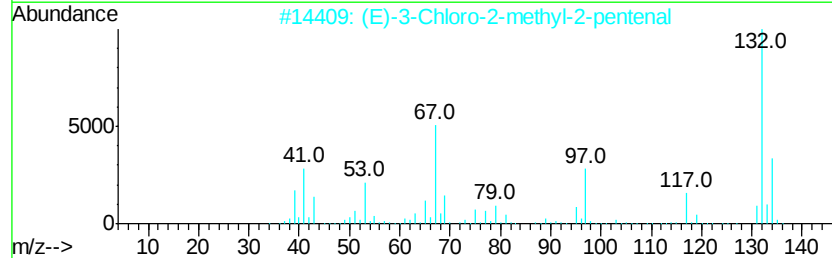
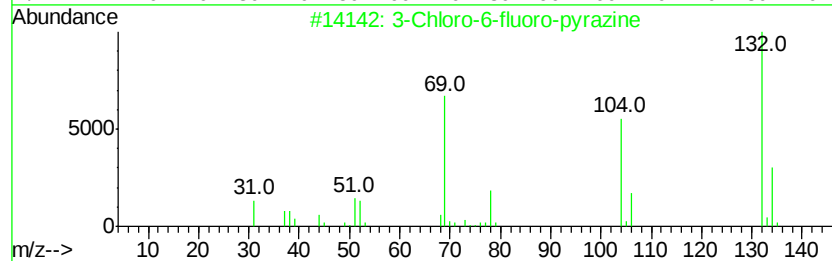
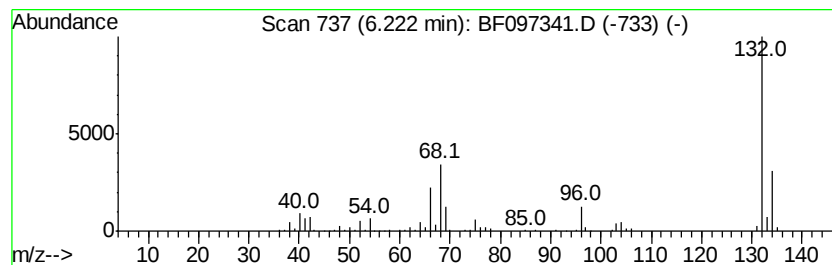
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

\*\*\*\*\*  
Peak Number 2 unknown6.22 Concentration Rank 1

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 6.22 | 16.33 ng | 476212 | 1,4-Dichlorobenzene-d4 | 6.45 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm   | CAS#         | Qual |
|------|----|---|-------------------------------------|-----|-----------|--------------|------|
| 1    |    |   | 3-Chloro-6-fluoro-pyrazine          | 132 | C4H2ClFN2 | 1000146-10-7 | 35   |
| 2    |    |   | (E)-3-Chloro-2-methyl-2-pentenal    | 132 | C6H9ClO   | 031357-76-3  | 17   |
| 3    |    |   | 5-Aminoindole                       | 132 | C8H8N2    | 005192-03-0  | 12   |
| 4    |    |   | 1-Methylpyrrolo[1,2-a]pyrazine      | 132 | C8H8N2    | 064608-59-9  | 9    |
| 5    |    |   | 2H-Cyclopenta[d]pyridazine, 2-me... | 132 | C8H8N2    | 022291-85-6  | 9    |



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Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF072517.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

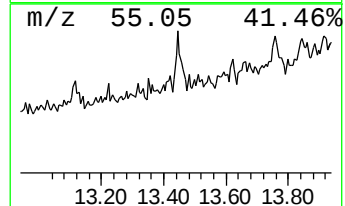
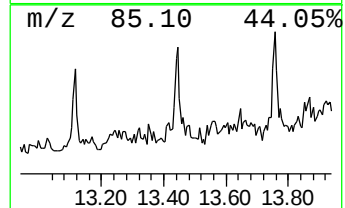
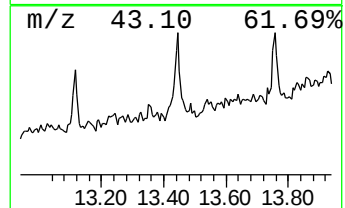
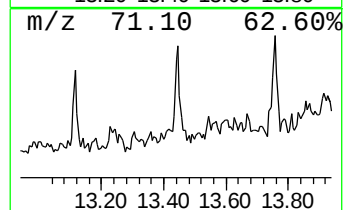
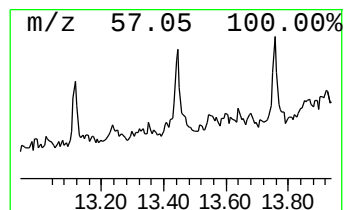
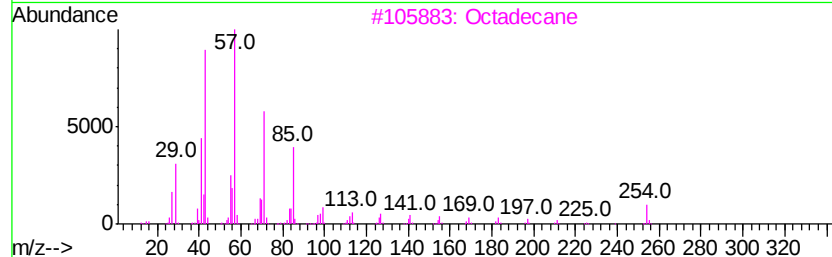
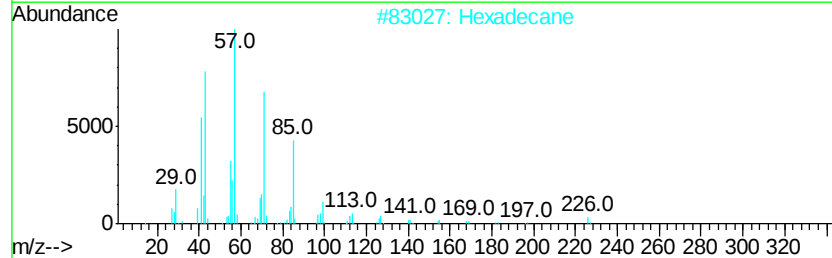
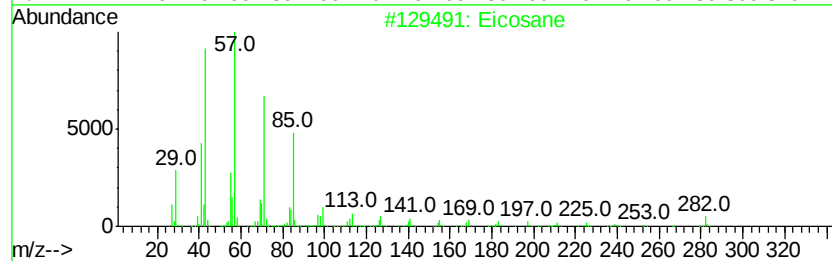
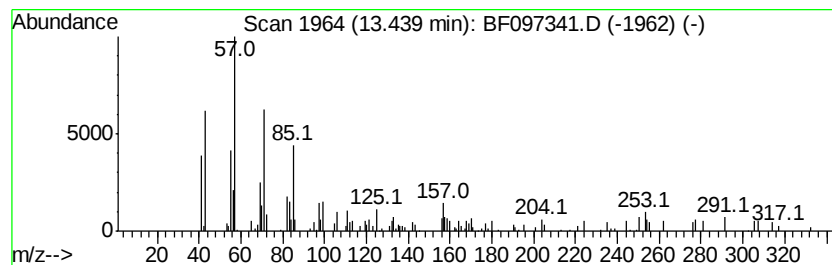
TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 4 Eicosane Concentration Rank 5

| R.T.  | EstConc | Area  | Relative to ISTD | R.T.  |
|-------|---------|-------|------------------|-------|
| 13.44 | 2.70 ng | 65086 | Chrysene-d12     | 13.56 |

| Hit# of | 5             | Tentative ID | MW  | MolForm | CAS#        | Qual |
|---------|---------------|--------------|-----|---------|-------------|------|
| 1       | Eicosane      |              | 282 | C20H42  | 000112-95-8 | 83   |
| 2       | Hexadecane    |              | 226 | C16H34  | 000544-76-3 | 78   |
| 3       | Octadecane    |              | 254 | C18H38  | 000593-45-3 | 58   |
| 4       | 5-Iodo-nonane |              | 254 | C9H19I  | 059456-19-8 | 58   |
| 5       | Undecane      |              | 156 | C11H24  | 001120-21-4 | 42   |



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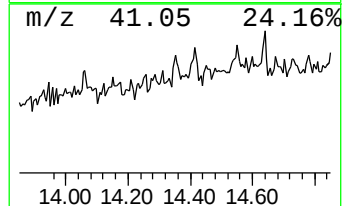
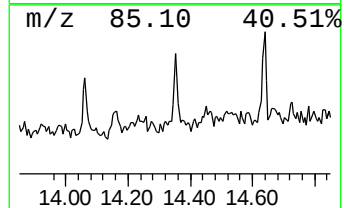
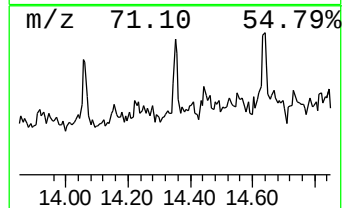
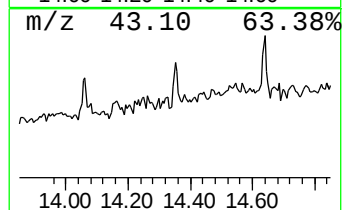
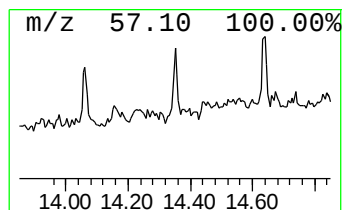
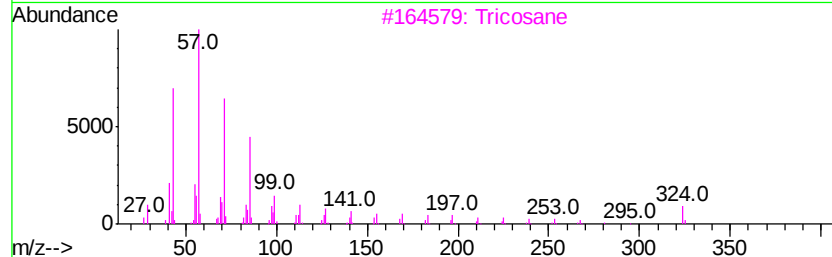
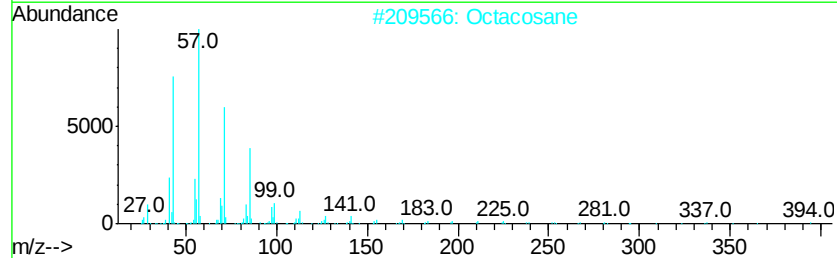
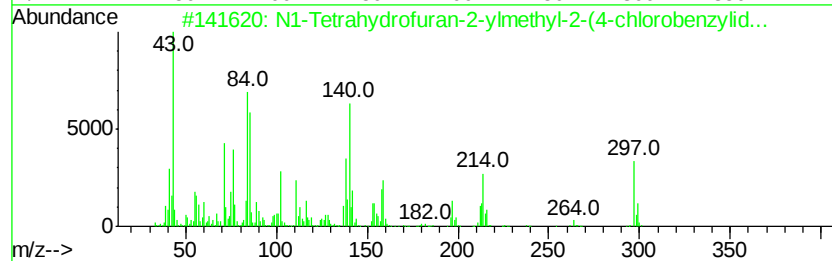
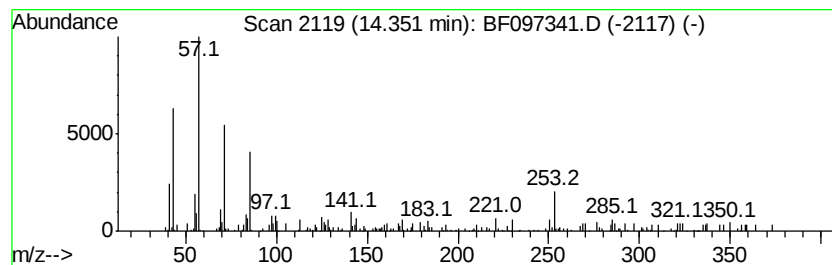
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TIC Library : C:\DATABASE\NIST11.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 5 N1-Tetrahydrofuran-2-ylmeth... Concentration Rank 4

| R.T.    | EstConc | Area                                | Relative to ISTD |              | R.T.        |      |
|---------|---------|-------------------------------------|------------------|--------------|-------------|------|
| 14.35   | 3.26 ng | 48274                               | Perylene-d12     |              | 14.91       |      |
| Hit# of | 5       | Tentative ID                        | MW               | MolForm      | CAS#        | Qual |
| 1       |         | N1-Tetrahydrofuran-2-ylmethyl-2-... | 297              | C13H16ClN3OS | 283155-62-4 | 86   |
| 2       |         | Octacosane                          | 394              | C28H58       | 000630-02-4 | 49   |
| 3       |         | Tricosane                           | 324              | C23H48       | 000638-67-5 | 49   |
| 4       |         | Pentacosane                         | 352              | C25H52       | 000629-99-2 | 47   |
| 5       |         | Nonadecane                          | 268              | C19H40       | 000629-92-5 | 47   |



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

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |        |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|--------|------|
|                      |       |         |       |          | #                     | RT    | Resp   | Conc |
| unknown6.22          | 6.22  | 16.3    | ng    | 476212   | 1                     | 6.45  | 583282 | 20.0 |
| Eicosane             | 13.44 | 2.7     | ng    | 65086    | 5                     | 13.56 | 481307 | 20.0 |
| N1-Tetrahydrofura... | 14.35 | 3.3     | ng    | 48274    | 6                     | 14.91 | 296163 | 20.0 |