

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
 Data File : BF085178.D  
 Acq On : 4 Mar 2016 1:25  
 Operator : SJ/UM  
 Sample : H1648-04  
 Misc :  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-47(COMP)

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-BF030316.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         | 5.190       | 251           | 254         | 260          | rVB      | 739068         | 993130        | 21.65%          | 1.572%        |
| 2         | 5.590       | 286           | 289         | 291          | rBV      | 3950646        | 4252418       | 92.68%          | 6.730%        |
| 3         | 6.607       | 374           | 378         | 380          | rBV      | 3121357        | 4588070       | 100.00%         | 7.261%        |
| 4         | 6.744       | 387           | 390         | 393          | rBV      | 4124938        | 4102072       | 89.41%          | 6.492%        |
| 5         | 6.939       | 405           | 407         | 408          | rBV      | 374735         | 539096        | 11.75%          | 0.853%        |
| 6         | 6.973       | 408           | 410         | 413          | rVV      | 1074358        | 1881273       | 41.00%          | 2.977%        |
| 7         | 7.064       | 413           | 418         | 419          | rVV5     | 295911         | 1014748       | 22.12%          | 1.606%        |
| 8         | 7.099       | 419           | 421         | 422          | rVV2     | 186251         | 370216        | 8.07%           | 0.586%        |
| 9         | 7.133       | 422           | 424         | 426          | rVV      | 3456722        | 3504202       | 76.38%          | 5.546%        |
| 10        | 7.167       | 426           | 427         | 430          | rVV3     | 57265          | 150807        | 3.29%           | 0.239%        |
| 11        | 7.419       | 447           | 449         | 451          | rVB3     | 81161          | 87913         | 1.92%           | 0.139%        |
| 12        | 7.545       | 457           | 460         | 462          | rVB      | 2382756        | 3173890       | 69.18%          | 5.023%        |
| 13        | 7.602       | 462           | 465         | 469          | rVB6     | 65198          | 169069        | 3.68%           | 0.268%        |
| 14        | 7.705       | 472           | 474         | 475          | rVB2     | 72516          | 70356         | 1.53%           | 0.111%        |
| 15        | 7.739       | 475           | 477         | 478          | rBV2     | 76456          | 95639         | 2.08%           | 0.151%        |
| 16        | 7.796       | 480           | 482         | 484          | rVV3     | 166365         | 281741        | 6.14%           | 0.446%        |
| 17        | 7.842       | 484           | 486         | 487          | rVB2     | 95389          | 87583         | 1.91%           | 0.139%        |
| 18        | 7.979       | 496           | 498         | 499          | rVV2     | 120593         | 116983        | 2.55%           | 0.185%        |
| 19        | 8.013       | 499           | 501         | 504          | rVB4     | 89582          | 158497        | 3.45%           | 0.251%        |
| 20        | 8.070       | 504           | 506         | 508          | rBV3     | 66323          | 98948         | 2.16%           | 0.157%        |
| 21        | 8.265       | 520           | 523         | 524          | rBV      | 1238160        | 1234501       | 26.91%          | 1.954%        |
| 22        | 8.287       | 524           | 525         | 527          | rVB2     | 91694          | 75868         | 1.65%           | 0.120%        |
| 23        | 8.345       | 528           | 530         | 532          | rBV3     | 87643          | 133924        | 2.92%           | 0.212%        |
| 24        | 8.482       | 540           | 542         | 545          | rVB4     | 79623          | 173653        | 3.78%           | 0.275%        |
| 25        | 8.539       | 545           | 547         | 548          | rVB2     | 101124         | 125053        | 2.73%           | 0.198%        |
| 26        | 8.585       | 548           | 551         | 552          | rBV3     | 131458         | 197733        | 4.31%           | 0.313%        |
| 27        | 8.676       | 557           | 559         | 560          | rBV2     | 66287          | 94053         | 2.05%           | 0.149%        |
| 28        | 8.950       | 581           | 583         | 584          | rVB2     | 83998          | 75596         | 1.65%           | 0.120%        |
| 29        | 8.996       | 584           | 587         | 591          | rBV6     | 92404          | 244236        | 5.32%           | 0.387%        |
| 30        | 9.236       | 605           | 608         | 610          | rVB4     | 106738         | 175389        | 3.82%           | 0.278%        |
| 31        | 9.339       | 615           | 617         | 619          | rVB      | 4808530        | 4501659       | 98.12%          | 7.124%        |
| 32        | 9.613       | 639           | 641         | 644          | rBV2     | 749160         | 1961015       | 42.74%          | 3.103%        |
| 33        | 9.728       | 649           | 651         | 655          | rVB      | 1099195        | 1508907       | 32.89%          | 2.388%        |
| 34        | 9.910       | 665           | 667         | 669          | rBV3     | 230964         | 551177        | 12.01%          | 0.872%        |

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
 Data File : BF085178.D  
 Acq On : 4 Mar 2016 1:25  
 Operator : SJ/UM  
 Sample : H1648-04  
 Misc :  
 ALS Vial : 22 Sample Multiplier: 1

Instrument :  
 BNA\_F  
 ClientSampleId :  
 SB-47(COMP)

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-BF030316.M  
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

|    |        |      |      |      |      |         |         |        |        |
|----|--------|------|------|------|------|---------|---------|--------|--------|
| 35 | 10.013 | 674  | 676  | 679  | rVB  | 1244487 | 1401398 | 30.54% | 2.218% |
| 36 | 10.151 | 684  | 688  | 689  | rBV4 | 417050  | 1101598 | 24.01% | 1.743% |
| 37 | 10.391 | 705  | 709  | 710  | rBV4 | 267527  | 997532  | 21.74% | 1.579% |
| 38 | 10.448 | 713  | 714  | 715  | rVV  | 759789  | 824125  | 17.96% | 1.304% |
| 39 | 10.482 | 715  | 717  | 719  | rVB2 | 776611  | 1057523 | 23.05% | 1.674% |
| 40 | 10.665 | 730  | 733  | 736  | rBV  | 67763   | 111713  | 2.43%  | 0.177% |
| 41 | 10.745 | 737  | 740  | 743  | rVV3 | 459524  | 1402595 | 30.57% | 2.220% |
| 42 | 10.802 | 743  | 745  | 751  | rVV  | 2498512 | 3844267 | 83.79% | 6.084% |
| 43 | 10.916 | 753  | 755  | 762  | rVB  | 229723  | 266316  | 5.80%  | 0.421% |
| 44 | 11.362 | 792  | 794  | 796  | rBV  | 77176   | 74368   | 1.62%  | 0.118% |
| 45 | 11.499 | 804  | 806  | 809  | rBV  | 1488238 | 1329862 | 28.99% | 2.105% |
| 46 | 11.568 | 809  | 812  | 815  | rVB2 | 46684   | 63837   | 1.39%  | 0.101% |
| 47 | 12.025 | 849  | 852  | 854  | rBV  | 28797   | 47169   | 1.03%  | 0.075% |
| 48 | 12.276 | 872  | 874  | 876  | rBV  | 68617   | 54418   | 1.19%  | 0.086% |
| 49 | 12.711 | 910  | 912  | 914  | rBV  | 61362   | 53368   | 1.16%  | 0.084% |
| 50 | 12.928 | 928  | 931  | 933  | rBV  | 267068  | 663770  | 14.47% | 1.050% |
| 51 | 12.985 | 933  | 936  | 937  | rVV2 | 300397  | 764203  | 16.66% | 1.209% |
| 52 | 13.031 | 938  | 940  | 942  | rVB2 | 300106  | 466064  | 10.16% | 0.738% |
| 53 | 13.088 | 942  | 945  | 947  | rBV  | 4335058 | 4194000 | 91.41% | 6.637% |
| 54 | 13.979 | 1020 | 1023 | 1028 | rBV  | 70853   | 110454  | 2.41%  | 0.175% |
| 55 | 14.139 | 1034 | 1037 | 1039 | rBV  | 791478  | 1006001 | 21.93% | 1.592% |
| 56 | 14.894 | 1099 | 1103 | 1109 | rBV2 | 25350   | 64336   | 1.40%  | 0.102% |
| 57 | 14.985 | 1109 | 1111 | 1114 | rVV  | 222906  | 224455  | 4.89%  | 0.355% |
| 58 | 15.602 | 1162 | 1165 | 1168 | rBV  | 535478  | 700829  | 15.28% | 1.109% |
| 59 | 16.048 | 1201 | 1204 | 1205 | rBV  | 445614  | 828645  | 18.06% | 1.311% |
| 60 | 16.323 | 1226 | 1228 | 1231 | rBV4 | 166995  | 493612  | 10.76% | 0.781% |
| 61 | 16.677 | 1257 | 1259 | 1264 | rVB2 | 34186   | 90957   | 1.98%  | 0.144% |
| 62 | 17.968 | 1369 | 1372 | 1373 | rBV2 | 566437  | 1253537 | 27.32% | 1.984% |
| 63 | 18.071 | 1380 | 1381 | 1384 | rVB2 | 625485  | 857559  | 18.69% | 1.357% |
| 64 | 18.163 | 1386 | 1389 | 1390 | rBV  | 397607  | 518200  | 11.29% | 0.820% |
| 65 | 18.208 | 1390 | 1393 | 1395 | rVV3 | 293065  | 659865  | 14.38% | 1.044% |
| 66 | 18.277 | 1395 | 1399 | 1400 | rVV3 | 156710  | 409880  | 8.93%  | 0.649% |
| 67 | 18.300 | 1400 | 1401 | 1402 | rVB  | 118119  | 97567   | 2.13%  | 0.154% |
| 68 | 18.437 | 1411 | 1413 | 1414 | rBV2 | 74253   | 131906  | 2.87%  | 0.209% |
| 69 | 19.466 | 1500 | 1503 | 1504 | rBV2 | 116251  | 232875  | 5.08%  | 0.369% |

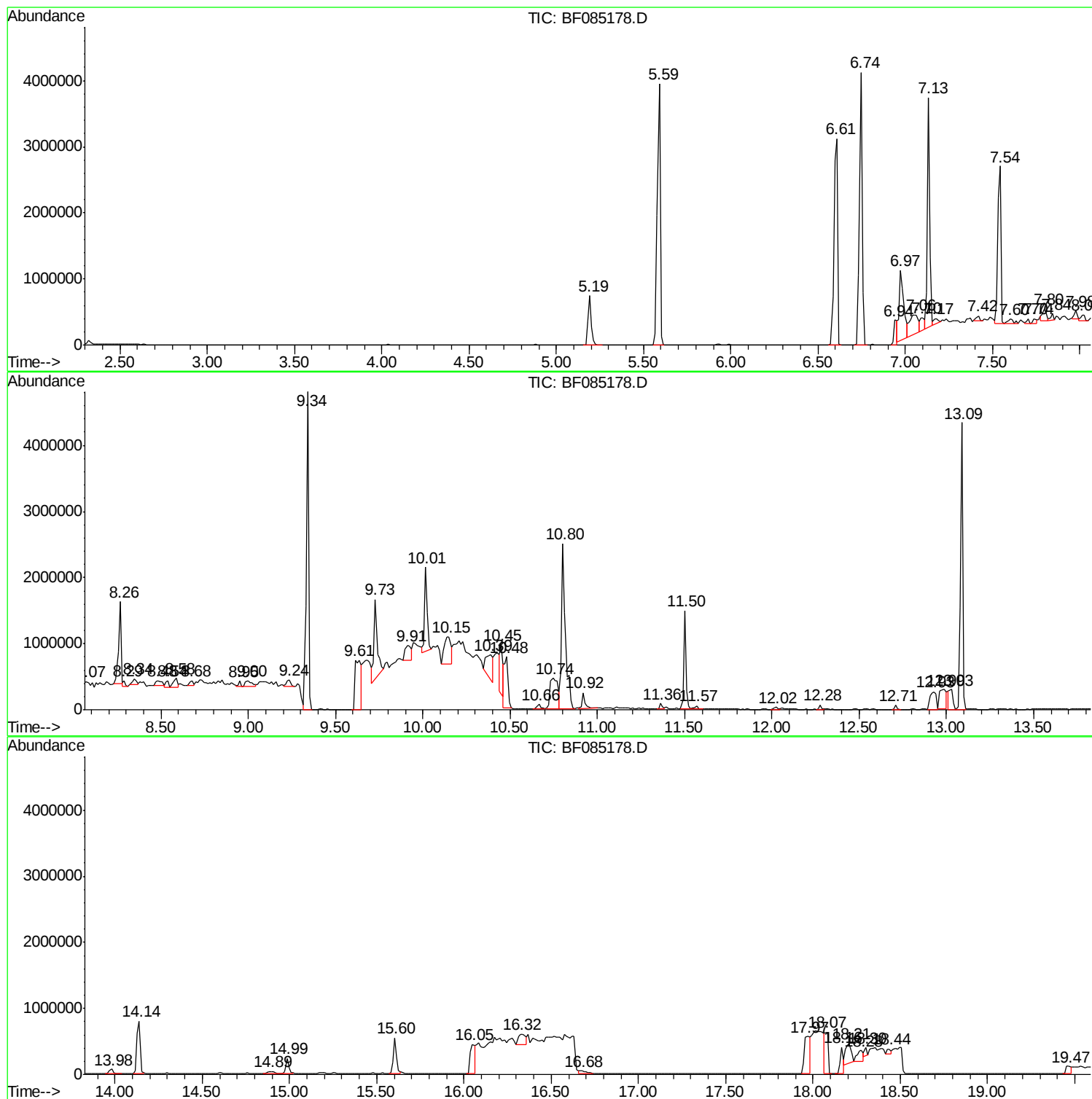
Sum of corrected areas: 63188219

Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

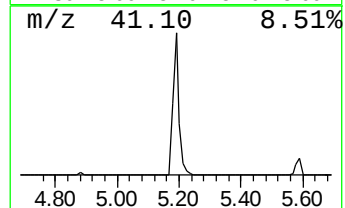
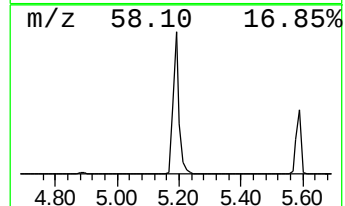
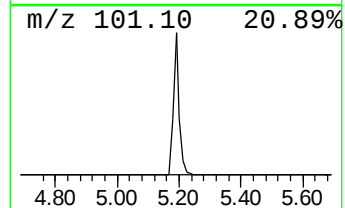
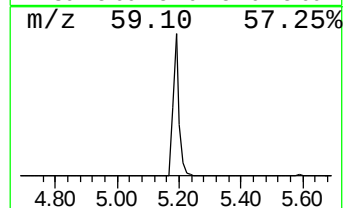
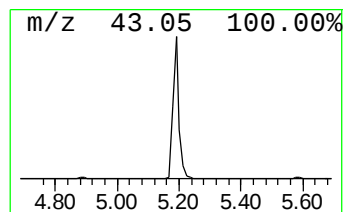
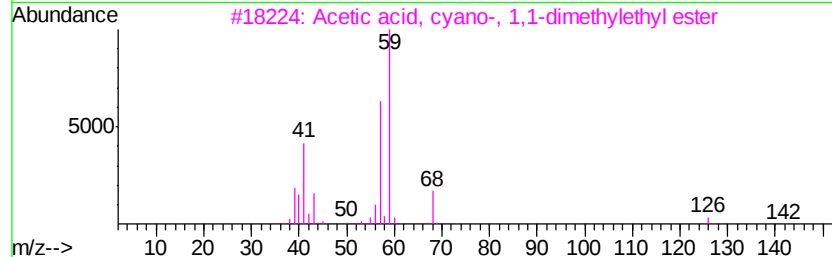
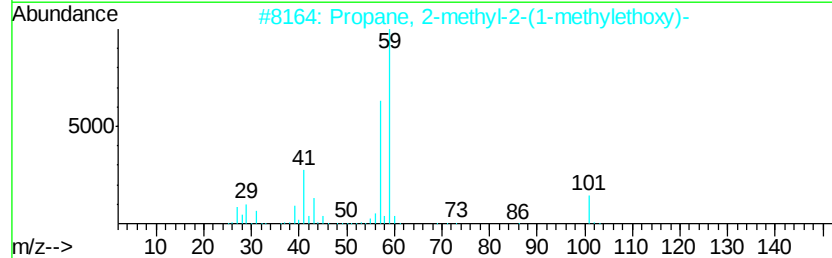
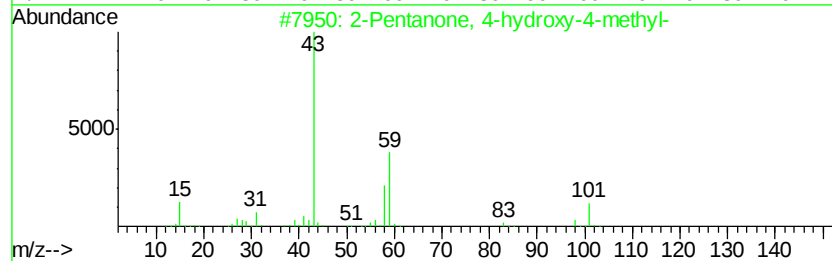
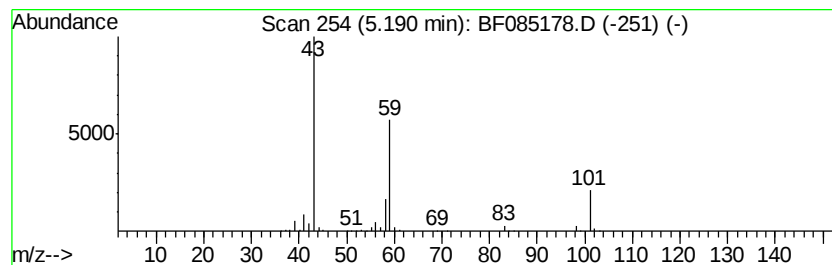
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 19

| R.T. | EstConc  | Area   | Relative to ISTD       | R.T. |
|------|----------|--------|------------------------|------|
| 5.19 | 10.56 ng | 993130 | 1,4-Dichlorobenzene-d4 | 6.97 |

| Hit# | of | 5 | Tentative ID                        | MW  | MolForm  | CAS#        | Qual |
|------|----|---|-------------------------------------|-----|----------|-------------|------|
| 1    |    |   | 2-Pentanone, 4-hydroxy-4-methyl-    | 116 | C6H12O2  | 000123-42-2 | 50   |
| 2    |    |   | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O   | 017348-59-3 | 23   |
| 3    |    |   | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23   |
| 4    |    |   | Butane, 1-ethoxy-                   | 102 | C6H14O   | 000628-81-9 | 9    |
| 5    |    |   | Morpholine, 4-methyl-               | 101 | C5H11NO  | 000109-02-4 | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

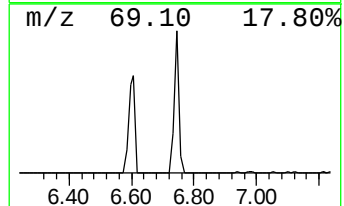
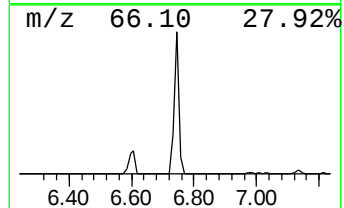
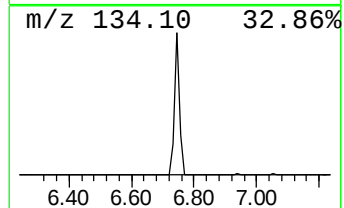
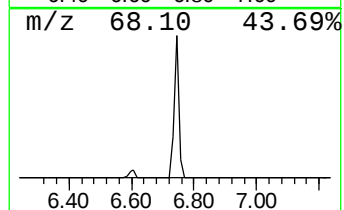
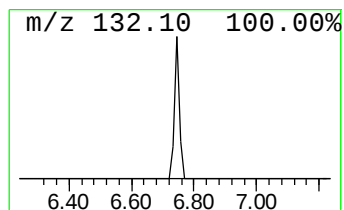
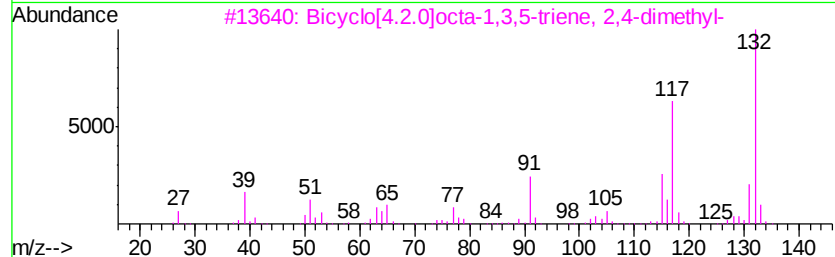
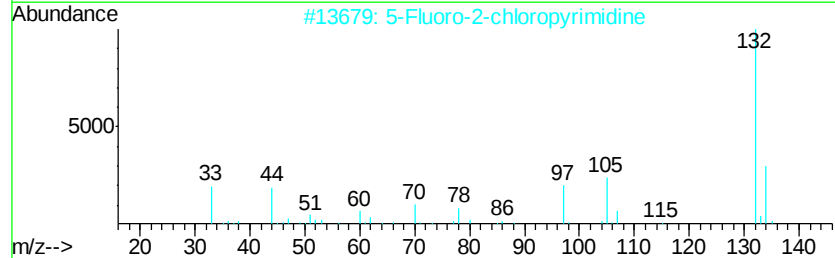
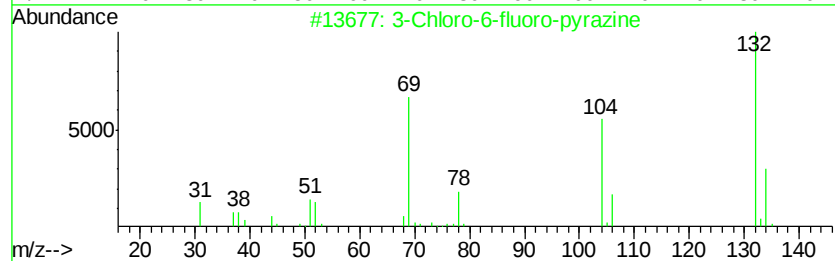
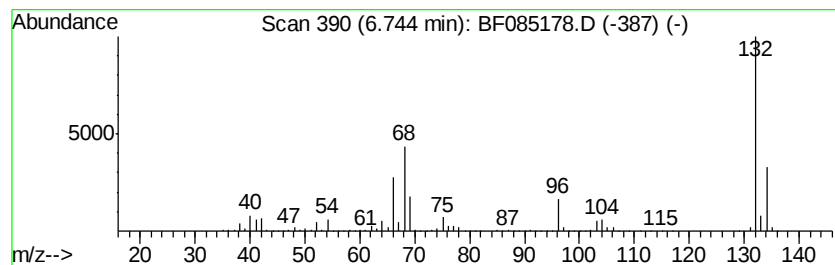
Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 2 unknown6.74 Concentration Rank 1

| R.T. | EstConc  | Area    | Relative to ISTD       | R.T. |
|------|----------|---------|------------------------|------|
| 6.74 | 43.61 ng | 4102070 | 1,4-Dichlorobenzene-d4 | 6.97 |

| 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  | 12   |
| 3    |    | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12    | 028749-81-7  | 9    |
| 4    |    | Benzene, 1-ethenyl-3,5-dimethyl-    | 132 | C10H12    | 005379-20-4  | 9    |
| 5    |    | 1,3,4-Thiadiazole-2(3H)-thione, ... | 132 | C3H4N2S2  | 029490-19-5  | 9    |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

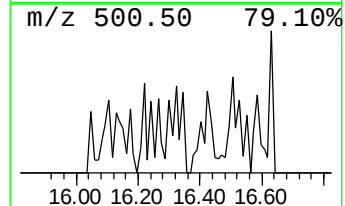
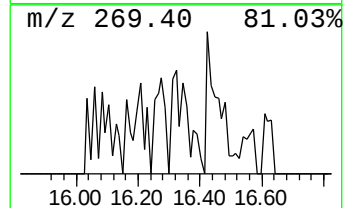
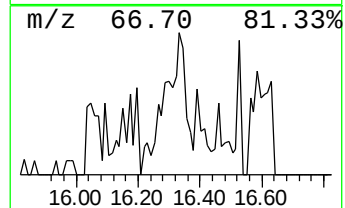
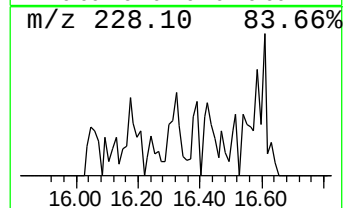
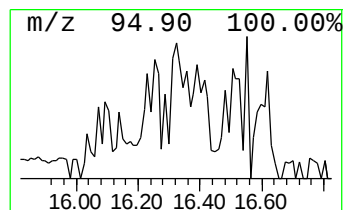
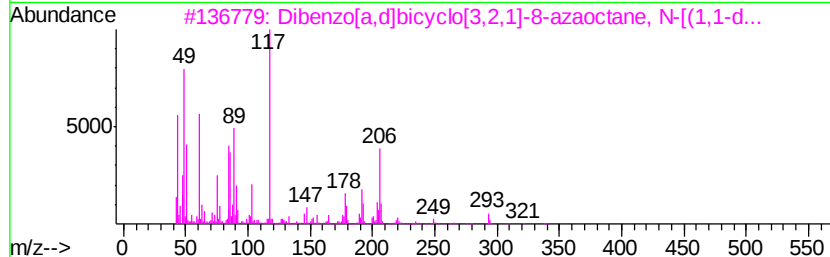
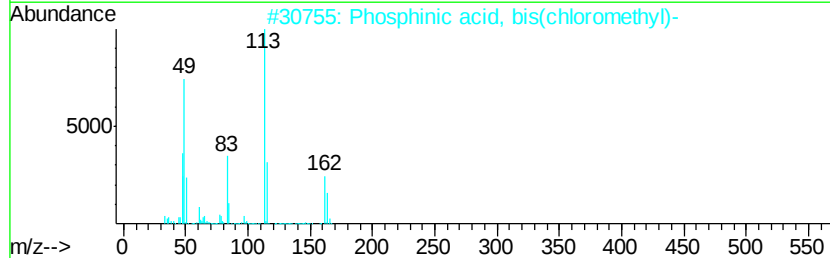
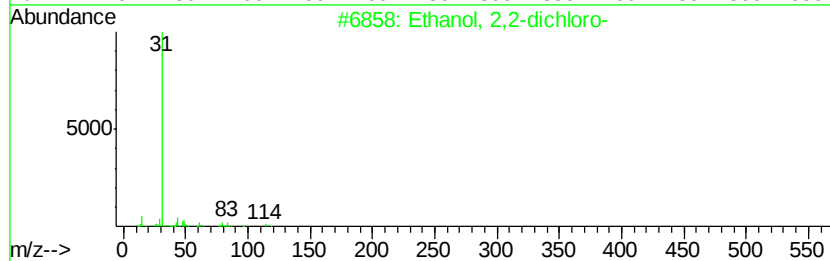
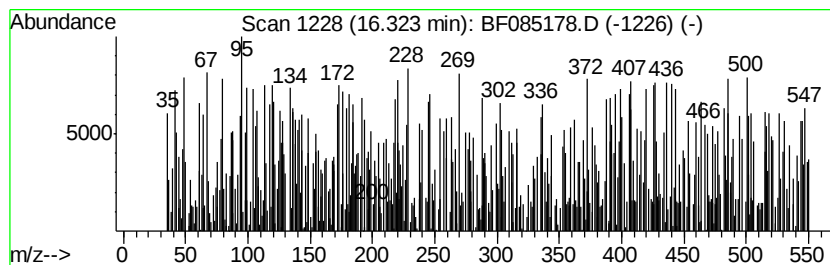
Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 15 unknown16.32 Concentration Rank 14

| R.T.    | EstConc                             | Area         | Relative to ISTD | R.T.            |
|---------|-------------------------------------|--------------|------------------|-----------------|
| 16.32   | 14.09 ng                            | 493612       | Perylene-d12     | 15.60           |
| Hit# of | 5                                   | Tentative ID | MW MolForm       | CAS# Qual       |
| 1       | Ethanol, 2,2-dichloro-              | 114          | C2H4Cl2O         | 000598-38-9 25  |
| 2       | Phosphinic acid, bis(chloromethyl)- | 162          | C2H5Cl2O2P       | 013274-83-4 22  |
| 3       | Dibenzo[a,d]bicyclo[3,2,1]-8-aza... | 339          | C21H25N03        | 1000128-43-4 13 |
| 4       | Imidazole-5-propionic acid, .bet... | 156          | C6H8N2O3         | 1000129-47-8 13 |
| 5       | 4"-Dehydroxy-2",3',3",4',5,6",7-... | 546          | C28H34O11        | 1000064-97-4 10 |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

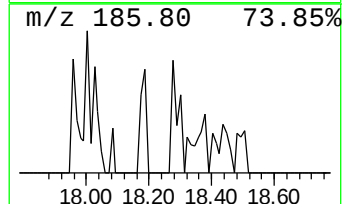
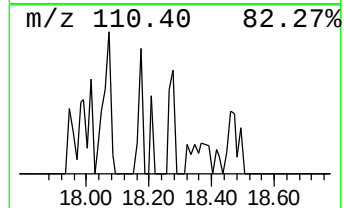
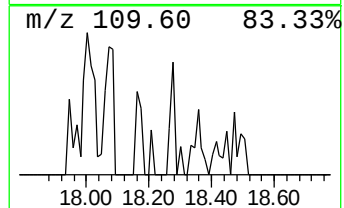
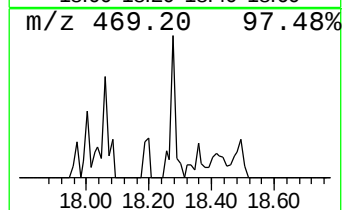
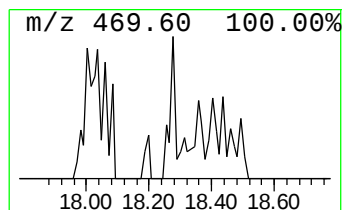
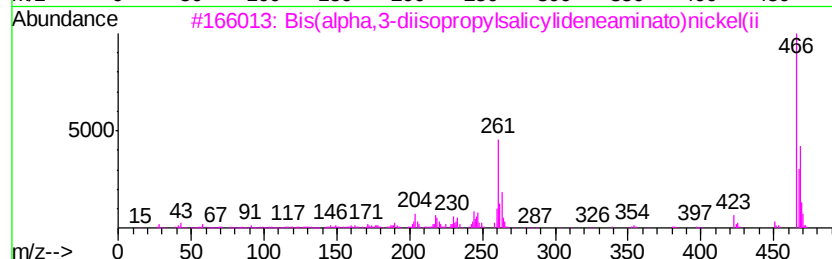
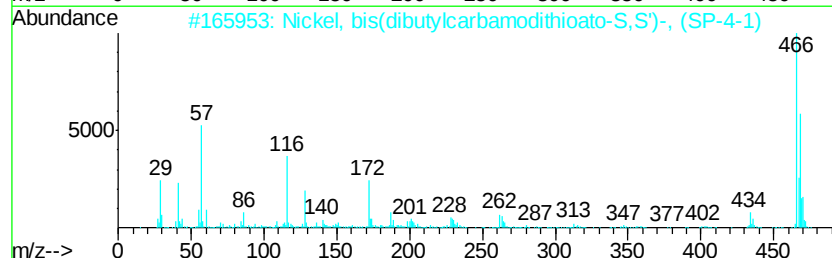
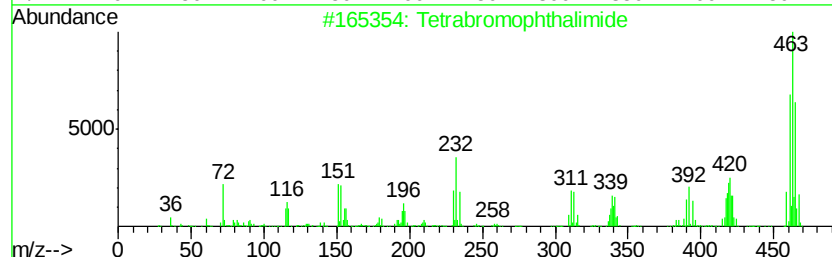
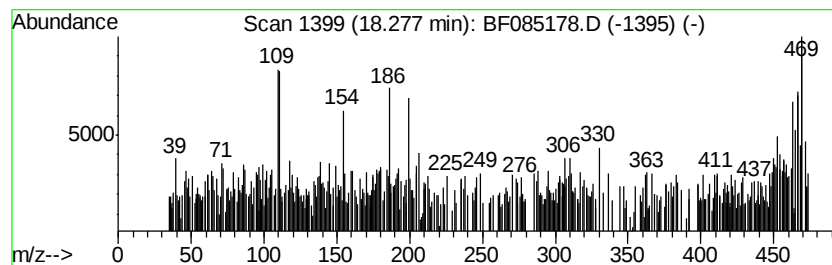
Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

\*\*\*\*\*  
Peak Number 20 unknown18.28 Concentration Rank 17

| R.T.    | EstConc  | Area                                | Relative to ISTD  | R.T.           |
|---------|----------|-------------------------------------|-------------------|----------------|
| 18.28   | 11.70 ng | 409880                              | Perylene-d12      | 15.60          |
| Hit# of | 5        | Tentative ID                        | MW MolForm        | CAS# Qual      |
| 1       |          | Tetrabromophthalimide               | 459 C8HBr4NO2     | 024407-32-7 25 |
| 2       |          | Nickel, bis(dibutylcarbamodithio... | 466 C18H36N2NiS4  | 013927-77-0 11 |
| 3       |          | Bis(alpha,3-diisopropylsalicylid... | 466 C26H36N2NiO2  | 025978-26-1 11 |
| 4       |          | 2,4,6(1H,3H,5H)-Pyrimidinetrione... | 463 C19H15BrFN3O5 | 333744-98-2 11 |
| 5       |          | [2,2](2,6)Naphthalenophane, 1,5-... | 464 C24H18Br2     | 1000149-74-9 9 |



Data Path : Z:\HPCHEM1\BNA\_F\DATA\BF030316\  
Data File : BF085178.D  
Acq On : 4 Mar 2016 1:25  
Operator : SJ/UM  
Sample : H1648-04  
Misc :  
ALS Vial : 22 Sample Multiplier: 1

Instrument :  
BNA\_F  
ClientSampleId :  
SB-47(COMP)

Quant Method : Z:\HPCHEM1\BNA\_F\METHODS\8270-BF030316.M  
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L  
TIC Integration Parameters: LSCINT.P

| TIC Top Hit name     | RT    | EstConc | Units | Response | --Internal Standard-- |       |         |      |
|----------------------|-------|---------|-------|----------|-----------------------|-------|---------|------|
|                      |       |         |       |          | #                     | RT    | Resp    | Conc |
| 2-Pentanone, 4-hy... | 5.19  | 10.6    | ng    | 993130   | 1                     | 6.97  | 1881270 | 20.0 |
| unknown6.74          | 6.74  | 43.6    | ng    | 4102070  | 1                     | 6.97  | 1881270 | 20.0 |
| unknown16.32         | 16.32 | 14.1    | ng    | 493612   | 6                     | 15.60 | 700829  | 20.0 |
| unknown18.28         | 18.28 | 11.7    | ng    | 409880   | 6                     | 15.60 | 700829  | 20.0 |