LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

| peak # | R.T. min | first scan | max scan | last scan | PK TY | peak height | corr. area | corr. % max. | % of total |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 2.155 | 3 | 6 | 7 | rBV | 1082058 | 1366605 | 2.76% | 0.458% |
| 2 | 2.178 | 7 | 8 | 13 | rVB | 502693 | 764121 | 1.54% | 0.256% |
| 3 | 3.070 | 80 | 86 | 89 | rBV3 | 276229 | 829552 | 1.68% | 0.278% |
| 4 | 3.493 | 112 | 123 | 125 | rBV3 | 198891 | 585902 | 1.18% | 0.196% |
| 5 | 3.630 | 130 | 135 | 139 | rBV2 | 336604 | 669613 | 1.35% | 0.224% |
| 6 | 4.350 | 197 | 198 | 200 | rVV | 443725 | 597721 | 1.21% | 0.200% |
| 7 | 4.453 | 203 | 207 | 208 | rVV | 640737 | 1039956 | 2.10% | 0.348% |
| 8 | 4.864 | 240 | 243 | 246 | rVB2 | 473830 | 560349 | 1.13% | 0.188% |
| 9 | 4.979 | 250 | 253 | 255 | rBV | 958034 | 1408651 | 2.84% | 0.472% |
| 10 | 5.081 | 260 | 262 | 265 | rVV2 | 1249411 | 2520828 | 5.09% | 0.844% |
| 11 | 5.139 | 265 | 267 | 271 | rVB2 | 766272 | 1697662 | 3.43% | 0.568% |
| 12 | 5.356 | 284 | 286 | 288 | rBV3 | 1414428 | 1716396 | 3.47% | 0.575% |
| 13 | 5.459 | 293 | 295 | 297 | rBV2 | 705987 | 1132767 | 2.29% | 0.379% |
| 14 | 5.504 | 297 | 299 | 302 | rVB | 4174236 | 4867367 | 9.83% | 1.630% |
| 15 | 5.630 | 306 | 310 | 311 | rBV3 | 474419 | 924182 | 1.87% | 0.309% |
| 16 | 5.676 | 311 | 314 | 317 | rVB3 | 501260 | 1020873 | 2.06% | 0.342% |
| 17 | 5.756 | 317 | 321 | 323 | rBV2 | 955552 | 1755058 | 3.54% | 0.588% |
| 18 | 5.802 | 323 | 325 | 327 | rVB | 2017511 | 1911896 | 3.86% | 0.640% |
| 19 | 5.836 | 327 | 328 | 331 | rVB2 | 525648 | 554480 | 1.12% | 0.186% |
| 20 | 5.904 | 331 | 334 | 336 | rBV | 1237959 | 2129779 | 4.30% | 0.713% |
| 21 | 5.950 | 336 | 338 | 340 | rVB | 2146107 | 1885543 | 3.81% | 0.631% |
| 22 | 6.019 | 342 | 344 | 346 | rBV2 | 2455229 | 3076695 | 6.21% | 1.030% |
| 23 | 6.053 | 346 | 347 | 349 | rVB | 1641283 | 1962253 | 3.96% | 0.657% |
| 24 | 6.099 | 349 | 351 | 356 | rVB | 2793681 | 3037320 | 6.13% | 1.017% |
| 25 | 6.213 | 358 | 361 | 365 | rBV5 | 737266 | 1800038 | 3.64% | 0.603% |
| 26 | 6.282 | 365 | 367 | 368 | rBV | 779462 | 1430861 | 2.89% | 0.479% |
| 27 | 6.304 | 368 | 369 | 372 | rVB3 | 1033494 | 1540714 | 3.11% | 0.516% |
| 28 | 6.442 | 375 | 381 | 383 | rBV2 | 4121075 | 4999618 | 10.10% | 1.674% |
| 29 | 6.487 | 384 | 385 | 387 | rVB2 | 474827 | 583807 | 1.18% | 0.195% |
| 30 | 6.567 | 387 | 392 | 393 | rBV | 2634722 | 4560037 | 9.21% | 1.527% |
| 31 | 6.613 | 393 | 396 | 398 | rVB | 1723209 | 2550464 | 5.15% | 0.854% |
| 32 | 6.670 | 398 | 401 | 404 | rBV | 5966906 | 9190522 | 18.56% | 3.077% |
| 33 | 6.739 | 404 | 407 | 408 | rBV3 | 517574 | 966059 | 1.95% | 0.323% |
| 34 | 6.773 | 408 | 410 | 415 | rVB3 | 688996 | 1169587 | 2.36% | 0.392% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 6.887 | 418 | 420 | 425 | rBV5 | 2308899 | 4911199 | 9.92% | 1.644% |
| 36 | 6.967 | 425 | 427 | 430 | rVB | 1924743 | 2707810 | 5.47% | 0.907% |
| 37 | 7.047 | 431 | 434 | 436 | rBV | 6521373 | 7764517 | 15.68% | 2.600% |
| 38 | 7.150 | 441 | 443 | 445 | rBV2 | 579150 | 927338 | 1.87% | 0.310% |
| 39 | 7.219 | 445 | 449 | 450 | rVB2 | 832907 | 1784576 | 3.60% | 0.597% |
| 40 | 7.345 | 454 | 460 | 463 | rBV2 | 17122776 | 49519251 | 100.00% | 16.579% |
| 41 | 7.402 | 463 | 465 | 467 | rBV | 675801 | 971099 | 1.96% | 0.325% |
| 42 | 7.459 | 467 | 470 | 473 | rBV2 | 6689199 | 12654129 | 25.55% | 4.237% |
| 43 | 7.550 | 475 | 478 | 479 | rBV | 866194 | 1732955 | 3.50% | 0.580% |
| 44 | 7.596 | 479 | 482 | 484 | rVB2 | 2371508 | 4609840 | 9.31% | 1.543% |
| 45 | 7.767 | 493 | 497 | 499 | rBV | 5212906 | 8874006 | 17.92% | 2.971% |
| 46 | 7.882 | 506 | 507 | 509 | rBV2 | 478922 | 692039 | 1.40% | 0.232% |
| 47 | 7.950 | 511 | 513 | 515 | rVV3 | 803305 | 1591733 | 3.21% | 0.533% |
| 48 | 8.007 | 515 | 518 | 520 | rVV2 | 7963557 | 13363658 | 26.99% | 4.474% |
| 49 | 8.053 | 520 | 522 | 524 | rVV2 | 1528996 | 1972590 | 3.98% | 0.660% |
| 50 | 8.099 | 524 | 526 | 527 | rVB2 | 549700 | 693399 | 1.40% | 0.232% |
| 51 | 8.179 | 527 | 533 | 537 | rBV4 | 2410468 | 7527042 | 15.20% | 2.520% |
| 52 | 8.305 | 541 | 544 | 547 | rVB3 | 496367 | 808265 | 1.63% | 0.271% |
| 53 | 8.362 | 547 | 549 | 550 | rBV | 909760 | 919979 | 1.86% | 0.308% |
| 54 | 8.453 | 553 | 557 | 558 | rBV | 2249464 | 3260349 | 6.58% | 1.092% |
| 55 | 8.488 | 558 | 560 | 562 | rVV2 | 3323116 | 3365106 | 6.80% | 1.127% |
| 56 | 8.556 | 565 | 566 | 568 | rVV2 | 1161998 | 1569462 | 3.17% | 0.525% |
| 57 | 8.648 | 568 | 574 | 577 | rVV5 | 1214832 | 4321908 | 8.73% | 1.447% |
| 58 | 8.739 | 581 | 582 | 583 | rBV | 488154 | 565849 | 1.14% | 0.189% |
| 59 | 8.773 | 583 | 585 | 587 | rVB2 | 1439651 | 1626433 | 3.28% | 0.545% |
| 60 | 8.830 | 587 | 590 | 592 | rBV3 | 398895 | 625435 | 1.26% | 0.209% |
| 61 | 8.888 | 592 | 595 | 597 | rBV2 | 600337 | 1229513 | 2.48% | 0.412% |
| 62 | 9.013 | 602 | 606 | 607 | rBV2 | 1057197 | 1452218 | 2.93% | 0.486% |
| 63 | 9.070 | 607 | 611 | 612 | rBV2 | 3853828 | 6653602 | 13.44% | 2.228% |
| 64 | 9.105 | 612 | 614 | 616 | rVB | 2673384 | 3321061 | 6.71% | 1.112% |
| 65 | 9.173 | 617 | 620 | 622 | rBV | 2246286 | 3148764 | 6.36% | 1.054% |
| 66 | 9.208 | 622 | 623 | 625 | rVV | 1464008 | 1251061 | 2.53% | 0.419% |
| 67 | 9.265 | 625 | 628 | 629 | rVV | 11042099 | 12047033 | 24.33% | 4.033% |
| 68 | 9.299 | 629 | 631 | 633 | rVB | 818816 | 1080519 | 2.18% | 0.362% |
| 69 | 9.368 | 633 | 637 | 640 | rVB | 2484831 | 4632920 | 9.36% | 1.551% |
| 70 | 9.482 | 644 | 647 | 649 | rBV2 | 660112 | 1045259 | 2.11% | 0.350% |
| 71 | 9.596 | 655 | 657 | 660 | rBV2 | 4487412 | 6000530 | 12.12% | 2.009% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

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-BF123115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 9.653 | 660 | 662 | 664 | rVV2 | 1807065 | 2304972 | 4.65% | 0.772% |
| 73 | 9.710 | 664 | 667 | 668 | rVB | 2292467 | 2671856 | 5.40% | 0.895% |
| 74 | 9.733 | 668 | 669 | 672 | rVB2 | 920101 | 1082564 | 2.19% | 0.362% |
| 75 | 9.825 | 672 | 677 | 679 | rBV5 | 694193 | 1830278 | 3.70% | 0.613% |
| 76 | 9.859 | 679 | 680 | 682 | rBV2 | 836777 | 1137552 | 2.30% | 0.381% |
| 77 | 9.939 | 684 | 687 | 689 | rVB2 | 4811266 | 4902306 | 9.90% | 1.641% |
| 78 | 10.019 | 691 | 694 | 695 | rVB2 | 585377 | 837718 | 1.69% | 0.280% |
| 79 | 10.076 | 697 | 699 | 700 | rBV2 | 1359289 | 1464577 | 2.96% | 0.490% |
| 80 | 10.099 | 700 | 701 | 705 | rVV3 | 1344100 | 1837545 | 3.71% | 0.615% |
| 81 | 10.191 | 707 | 709 | 710 | rBV | 796614 | 674562 | 1.36% | 0.226% |
| 82 | 10.385 | 723 | 726 | 728 | rVV3 | 560564 | 984842 | 1.99% | 0.330% |
| 83 | 10.568 | 738 | 742 | 746 | rVB5 | 1013818 | 2171391 | 4.38% | 0.727% |
| 84 | 10.648 | 747 | 749 | 752 | rBV3 | 318649 | 896561 | 1.81% | 0.300% |
| 85 | 10.728 | 754 | 756 | 759 | rVV | 5734645 | 6173240 | 12.47% | 2.067% |
| 86 | 10.842 | 765 | 766 | 771 | rVV3 | 426920 | 655002 | 1.32% | 0.219% |
| 87 | 10.933 | 772 | 774 | 776 | rVV2 | 422939 | 571123 | 1.15% | 0.191% |
| 88 | 11.048 | 782 | 784 | 786 | rVV2 | 983156 | 1101437 | 2.22% | 0.369% |
| 89 | 11.082 | 786 | 787 | 791 | rVV2 | 277120 | 539768 | 1.09% | 0.181% |
| 90 | 11.162 | 792 | 794 | 797 | rVB4 | 288316 | 552497 | 1.12% | 0.185% |
| 91 | 11.425 | 814 | 817 | 819 | rVB | 2180977 | 2689549 | 5.43% | 0.900% |
| 92 | 11.596 | 830 | 832 | 833 | rVB | 803756 | 944291 | 1.91% | 0.316% |
| 93 | 13.002 | 953 | 955 | 958 | rBV | 5049841 | 6248225 | 12.62% | 2.092% |
| 94 | 13.894 | 1032 | 1033 | 1035 | rVV | 355847 | 540646 | 1.09% | 0.181% |
| 95 | 13.928 | 1035 | 1036 | 1039 | rVB | 880880 | 732238 | 1.48% | 0.245% |
| 96 | 14.054 | 1045 | 1047 | 1049 | rBV | 2091214 | 1895261 | 3.83% | 0.635% |
| 97 | 15.494 | 1170 | 1173 | 1175 | rVB | 936802 | 1131918 | 2.29% | 0.379% |
| 98 | 16.134 | 1226 | 1229 | 1238 | rVB | 549912 | 1131271 | 2.28% | 0.379% |
| 99 | 17.197 | 1317 | 1322 | 1331 | rVB | 740488 | 1767584 | 3.57% | 0.592% |
| 100 | 18.637 | 1442 | 1448 | 1458 | rBV | 349003 | 1178469 | 2.38% | 0.395% |

Sum of corrected areas: 298678966

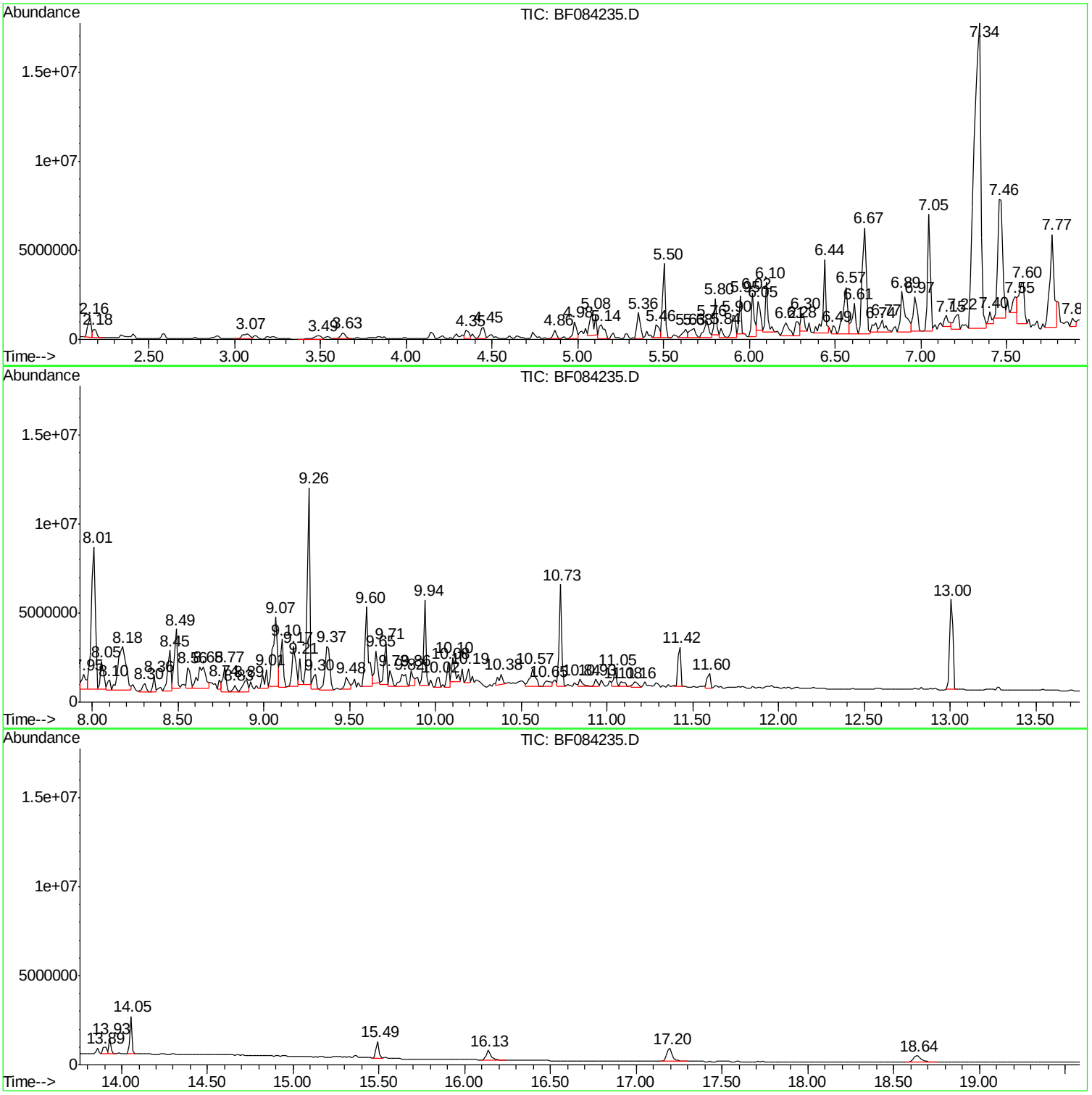
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.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\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

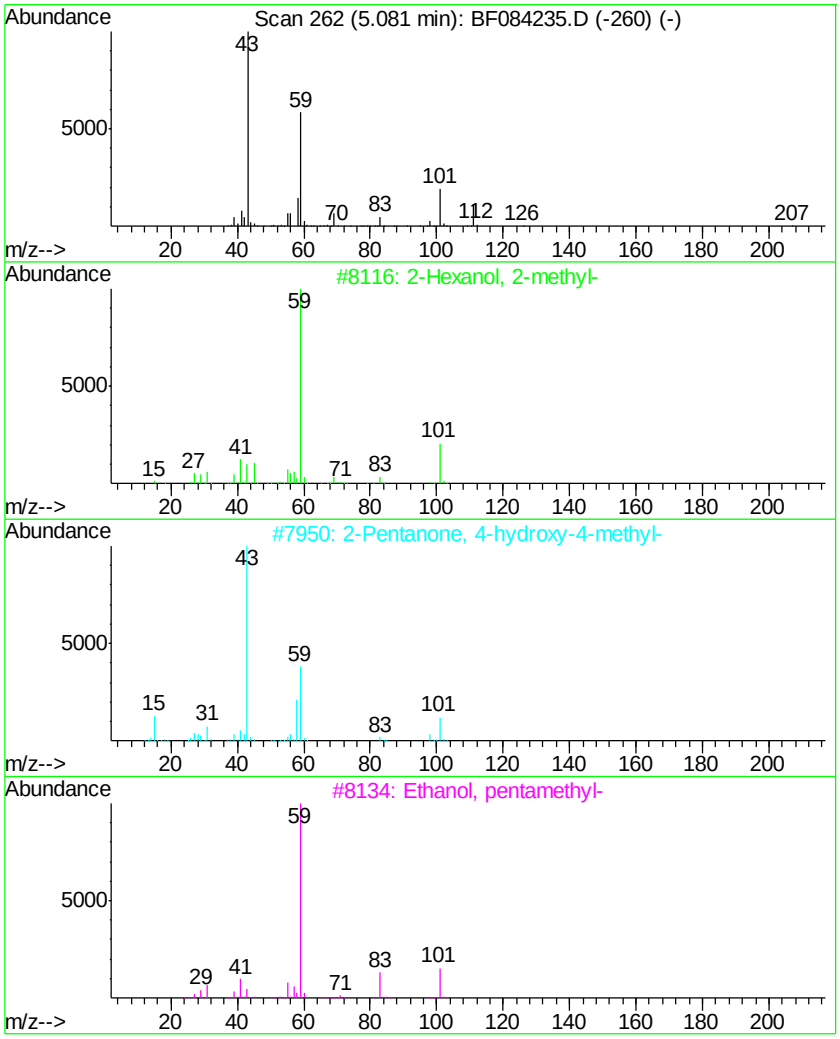
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

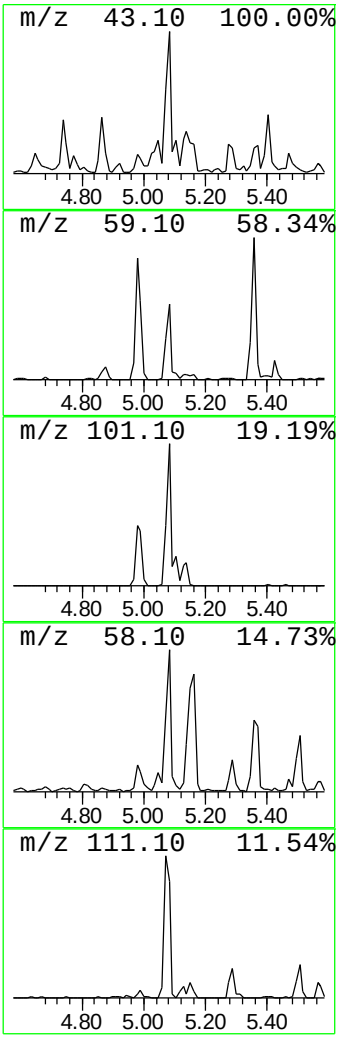
**********

Peak Number 1 unknown5.08 Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.08 | 10.27 ng | 2520830 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Hexanol, 2-methyl- | 116 | C7H16O | 000625-23-0 | 38 |
| 2 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 38 |
| 3 | Ethanol, pentamethyl- | 116 | C7H16O | 000594-83-2 | 28 |
| 4 | 3-Octanol | 130 | C8H18O | 020296-29-1 | 25 |
| 5 | 1,8-Nonanediol, 8-methyl- | 174 | C10H22O2 | 054725-73-4 | 23 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

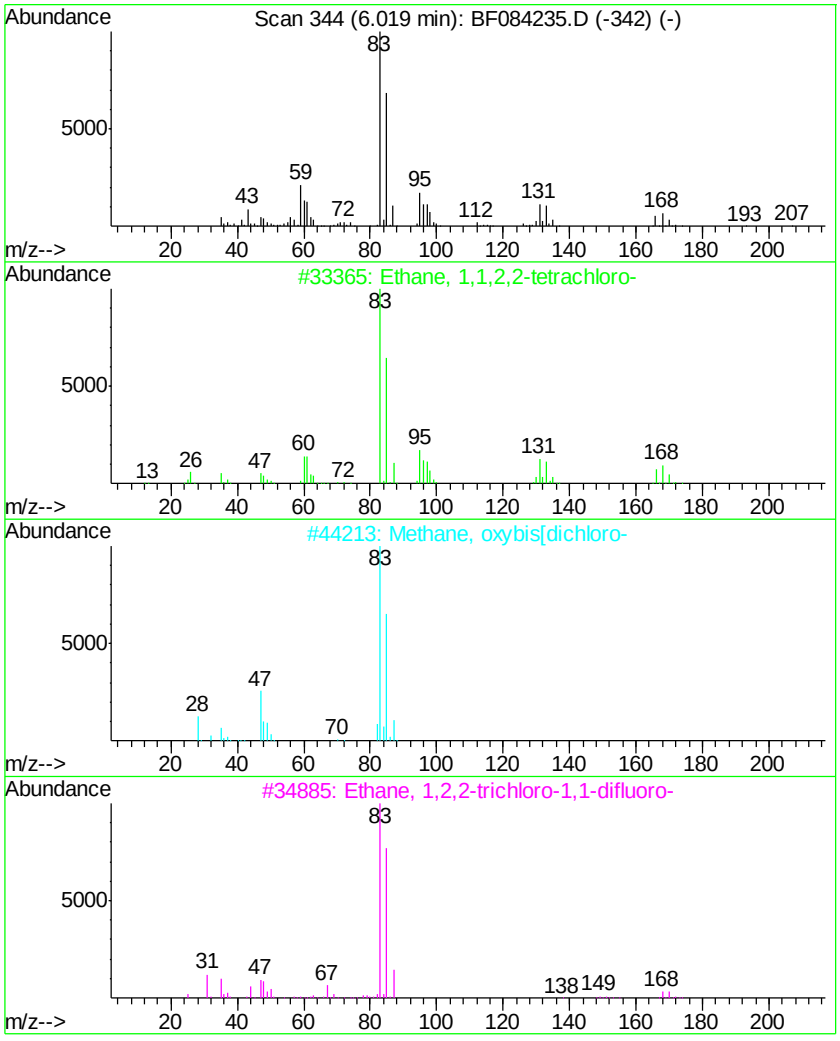
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

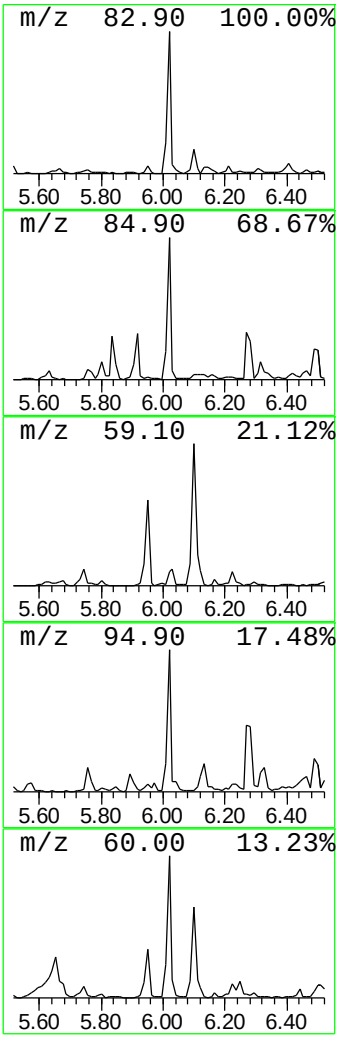
**********

Peak Number 2 Ethane, 1,1,2,2-tetrachloro- Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.02 | 12.53 ng | 3076700 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethane, 1,1,2,2-tetrachloro- | 166 | C2H2Cl4 | 000079-34-5 | 98 |
| 2 | Methane, oxybis[dichloro- | 182 | C2H2Cl4O | 020524-86-1 | 50 |
| 3 | Ethane, 1,2,2-trichloro-1,1-difl... | 168 | C2HCl3F2 | 000354-21-2 | 49 |
| 4 | Methane, bromodichloro- | 162 | CHBrCl2 | 000075-27-4 | 47 |
| 5 | Trichloromethane | 118 | CHCl3 | 000067-66-3 | 47 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

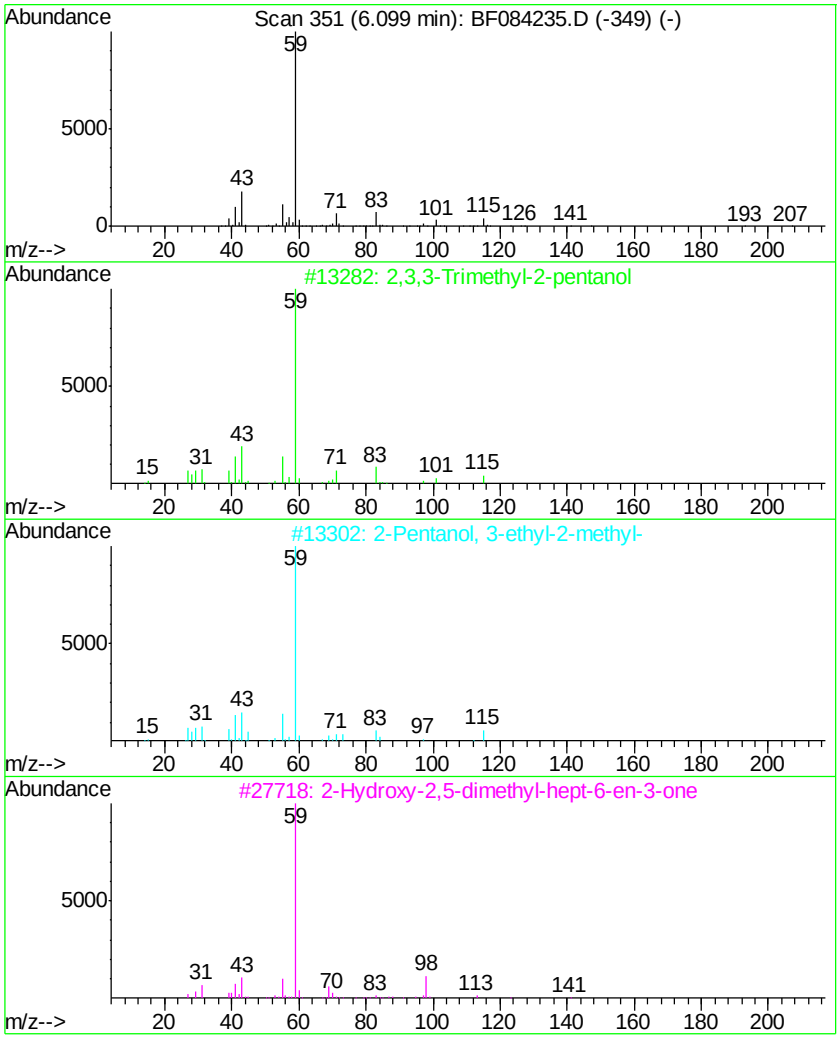
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

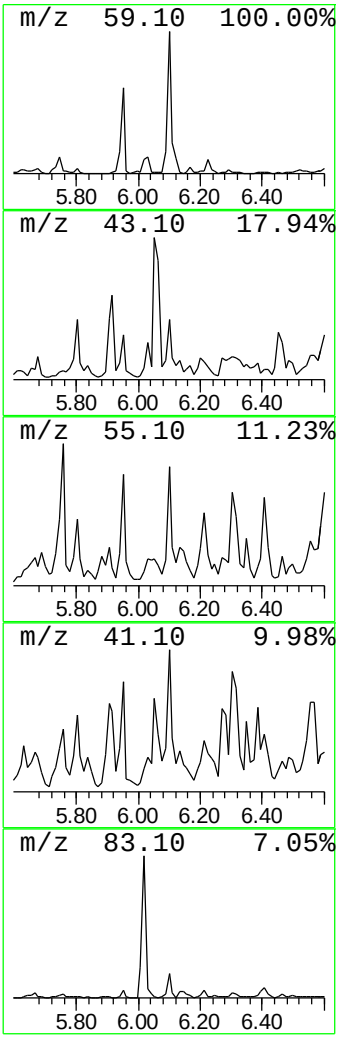
**********

Peak Number 3 2,3,3-Trimethyl-2-pentanol Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.10 | 12.37 ng | 3037320 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,3,3-Trimethyl-2-pentanol | 130 | C8H18O | 023171-85-9 | 78 |
| 2 | 2-Pentanol, 3-ethyl-2-methyl- | 130 | C8H18O | 019780-63-3 | 64 |
| 3 | 2-Hydroxy-2,5-dimethyl-hept-6-en... | 156 | C9H16O2 | 1000192-55-8 | 42 |
| 4 | 1-Butanol, 3-methoxy- | 104 | C5H12O2 | 002517-43-3 | 39 |
| 5 | Propanoic acid, 2-nitro-, methyl... | 133 | C4H7NO4 | 006118-50-9 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

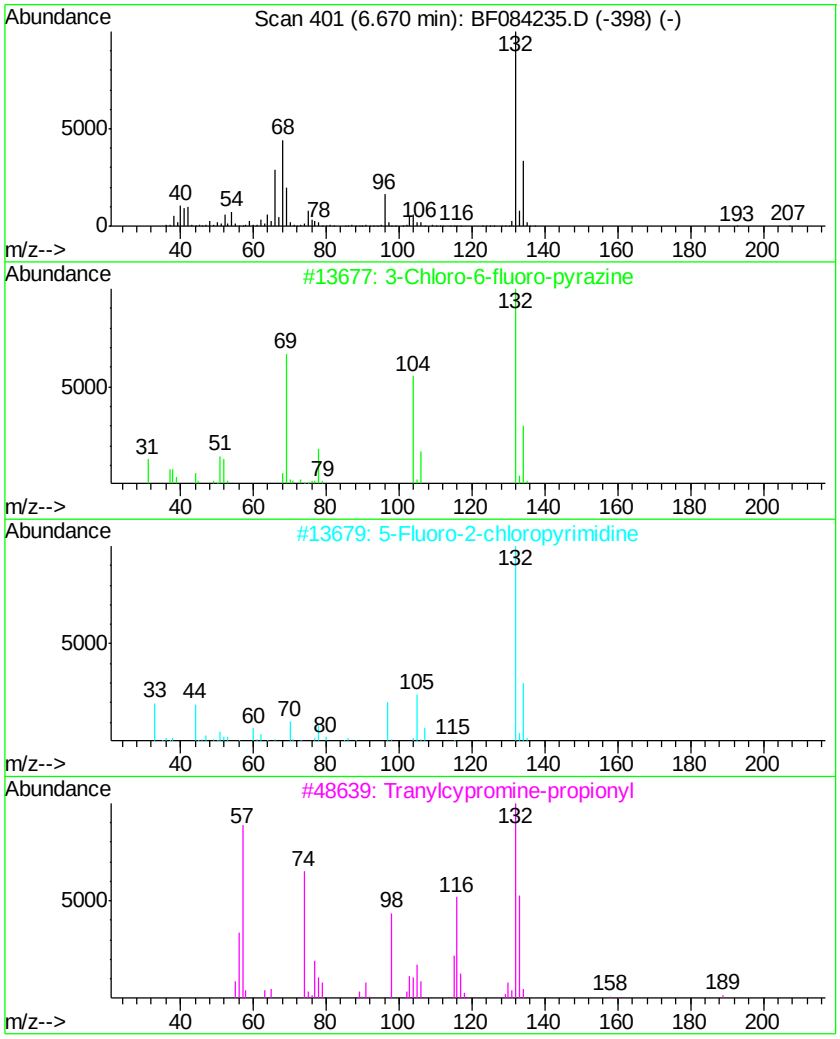
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

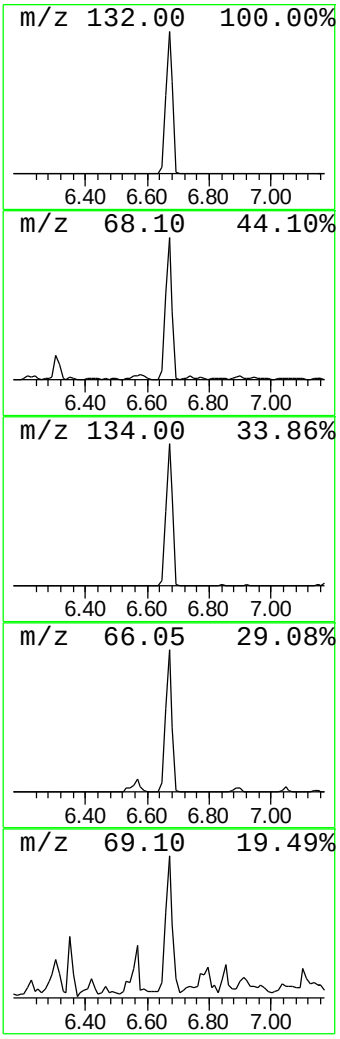
**********

Peak Number 4 unknown6.67 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.67 | 37.43 ng | 9190520 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 12 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | Benzene, 1,2,4-trifluoro- | 132 | C6H3F3 | 000367-23-7 | 9 |
| 5 | Benzene, 1,3,5-trifluoro- | 132 | C6H3F3 | 000372-38-3 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

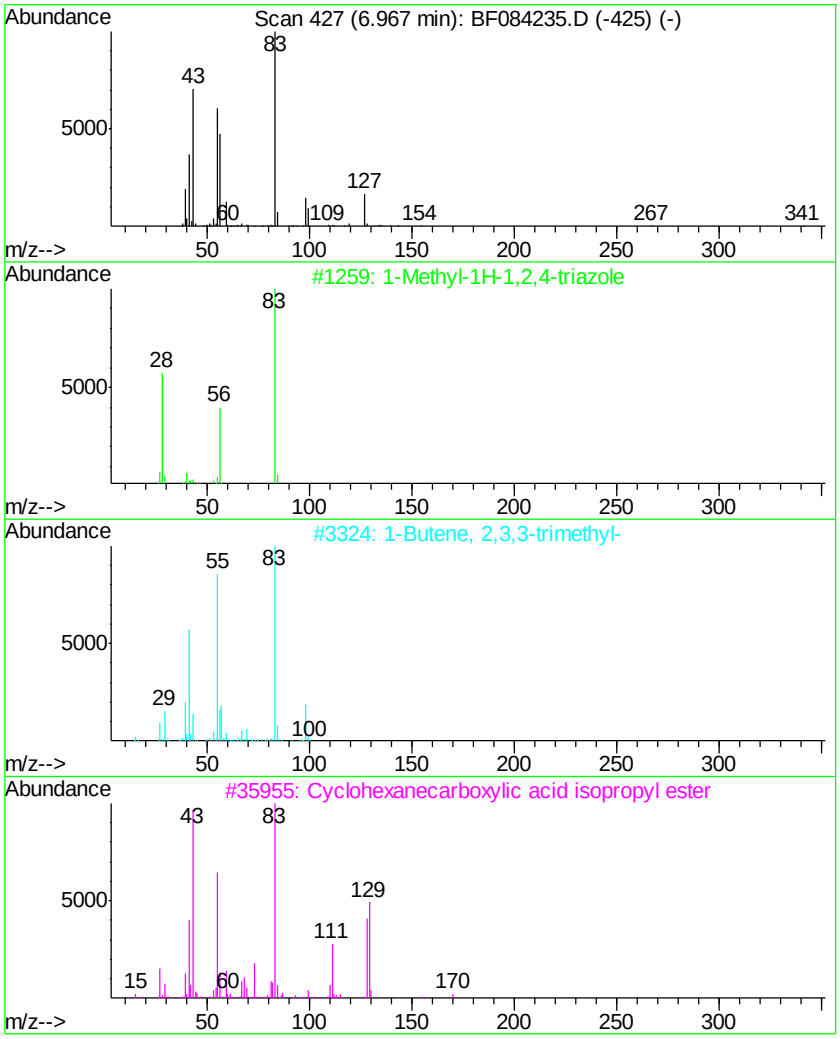
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

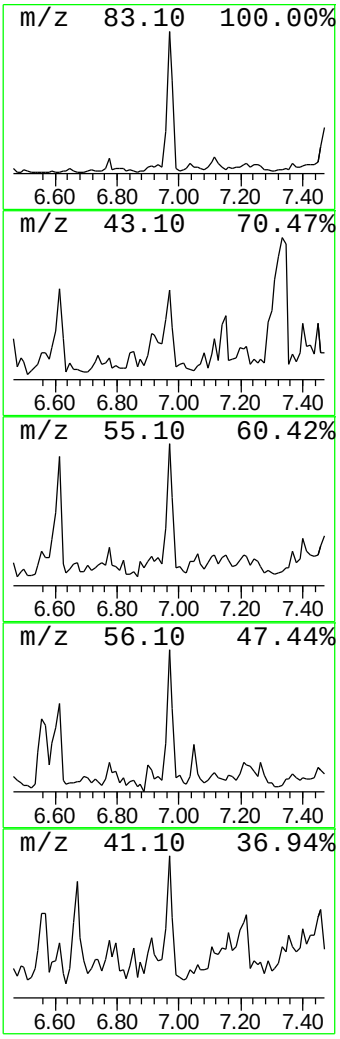
**********

Peak Number 5 1-Methyl-1H-1,2,4-triazole Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.97 | 11.03 ng | 2707810 | 1,4-Dichlorobenzene-d4 | 6.89 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Methyl-1H-1,2,4-triazole | 83 | C3H5N3 | 006086-21-1 | 53 |
| 2 | 1-Butene, 2,3,3-trimethyl- | 98 | C7H14 | 000594-56-9 | 35 |
| 3 | Cyclohexanecarboxylic acid isopr... | 170 | C10H18O2 | 006553-80-6 | 33 |
| 4 | 2-Pentene, 4,4-dimethyl-, (E)- | 98 | C7H14 | 000690-08-4 | 27 |
| 5 | Cyclopropane, 1,1,2,2-tetramethyl- | 98 | C7H14 | 004127-47-3 | 12 |



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Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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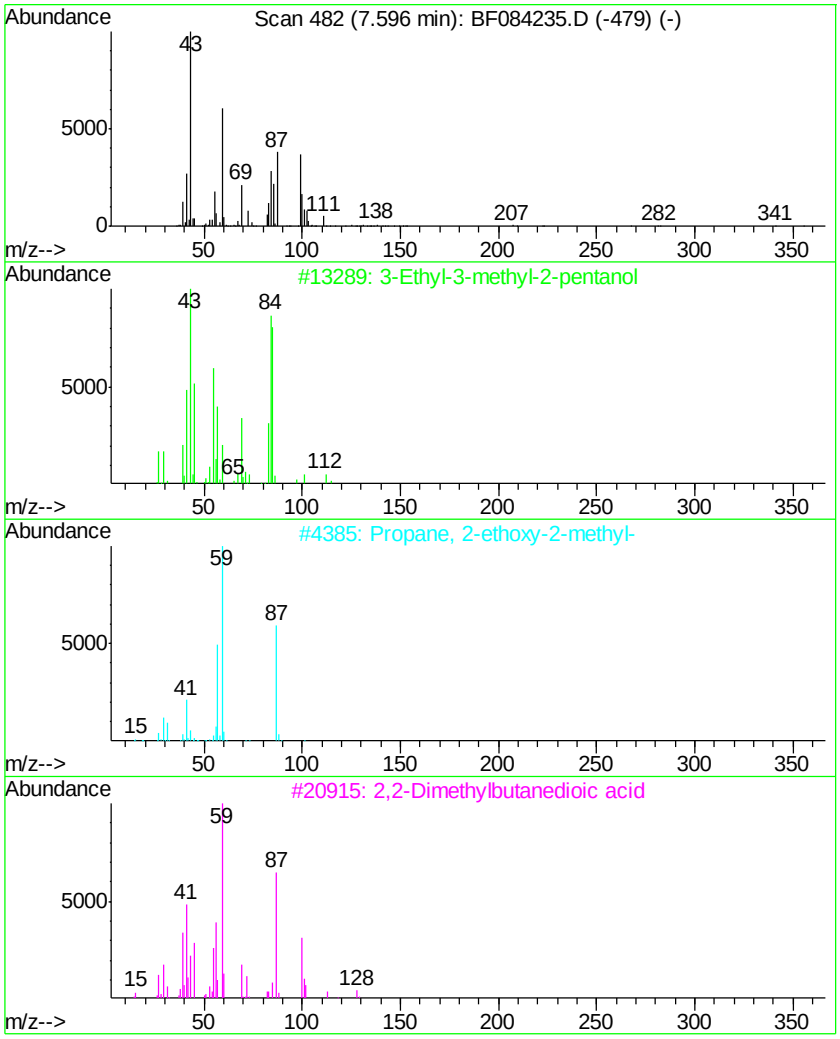
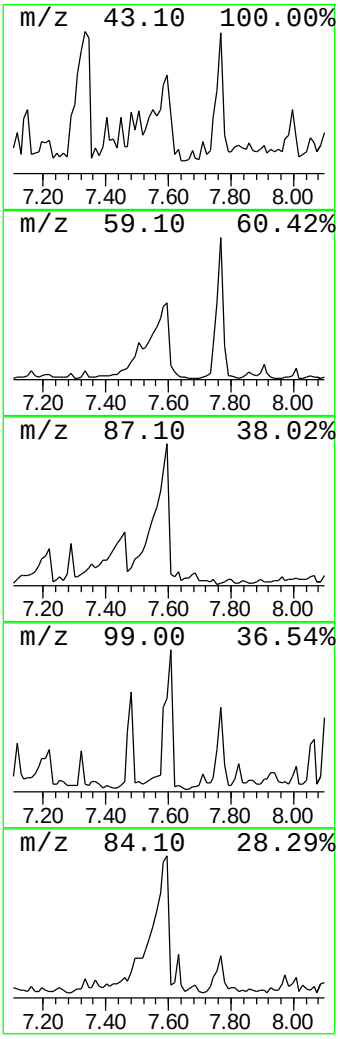
Peak Number 7 unknown7.60 Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.60 | 12.25 ng | 4609840 | Naphthalene-d8 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Ethyl-3-methyl-2-pentanol | 130 | C8H18O | 066576-22-5 | 22 |
| 2 | Propane, 2-ethoxy-2-methyl- | 102 | C6H14O | 000637-92-3 | 22 |
| 3 | 2,2-Dimethylbutanedioic acid | 146 | C6H10O4 | 000597-43-3 | 17 |
| 4 | Butane, 2-ethoxy-2-methyl- | 116 | C7H16O | 000919-94-8 | 16 |
| 5 | 4-Methyl-2-pentyl acetate | 144 | C8H16O2 | 000108-84-9 | 12 |



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Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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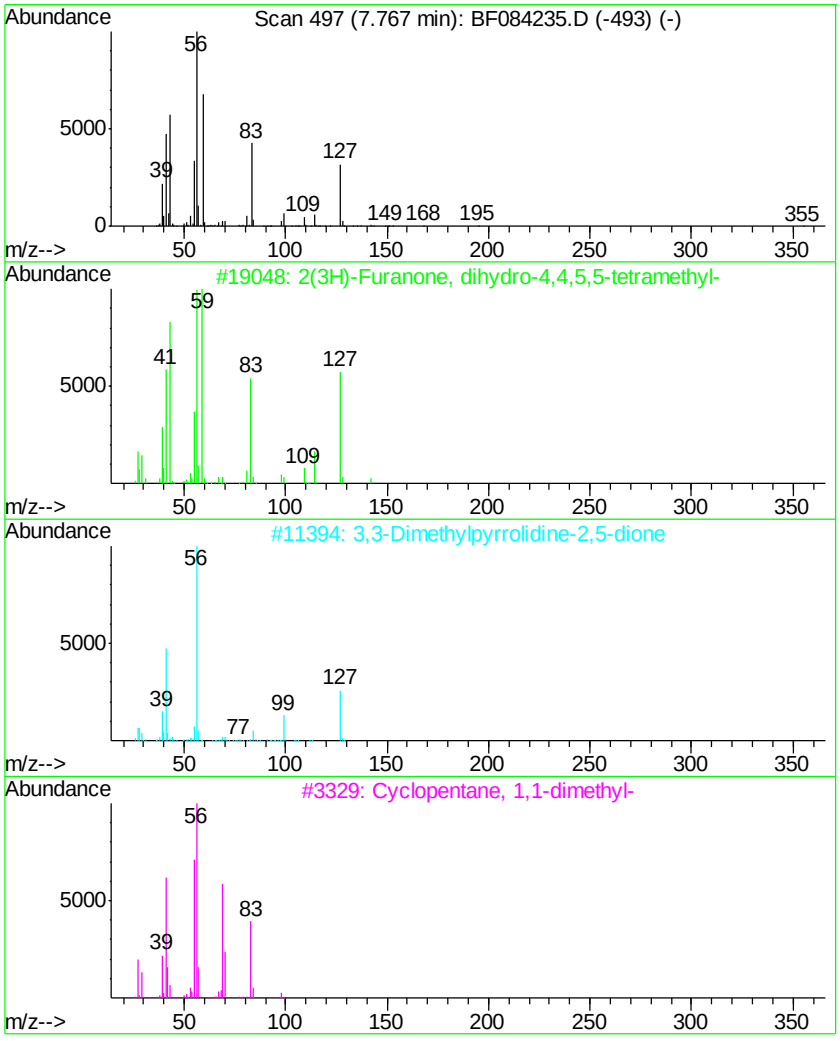
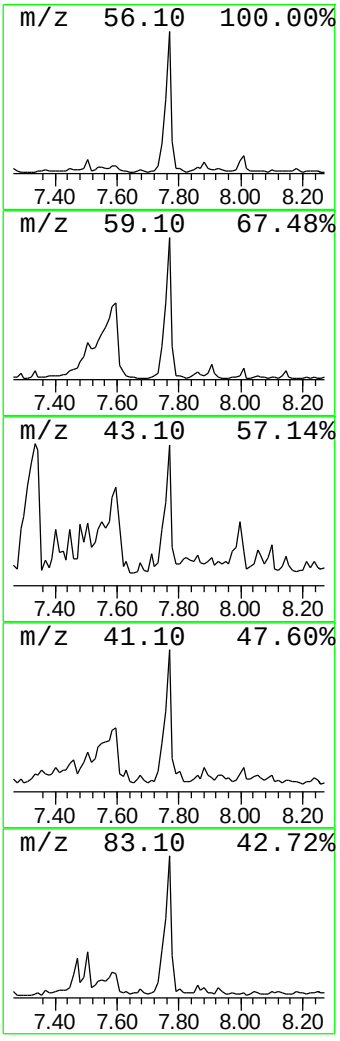
Peak Number 8 unknown7.77 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.77 | 23.58 ng | 8874010 | Naphthalene-d8 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2(3H)-Furanone, dihydro-4,4,5,5-... | 142 | C8H14O2 | 016466-24-3 | 45 |
| 2 | 3,3-Dimethylpyrrolidine-2,5-dione | 127 | C6H9NO2 | 003437-29-4 | 43 |
| 3 | Cyclopentane, 1,1-dimethyl- | 98 | C7H14 | 001638-26-2 | 37 |
| 4 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 35 |
| 5 | 1-Hexene, 2-methyl- | 98 | C7H14 | 006094-02-6 | 30 |



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Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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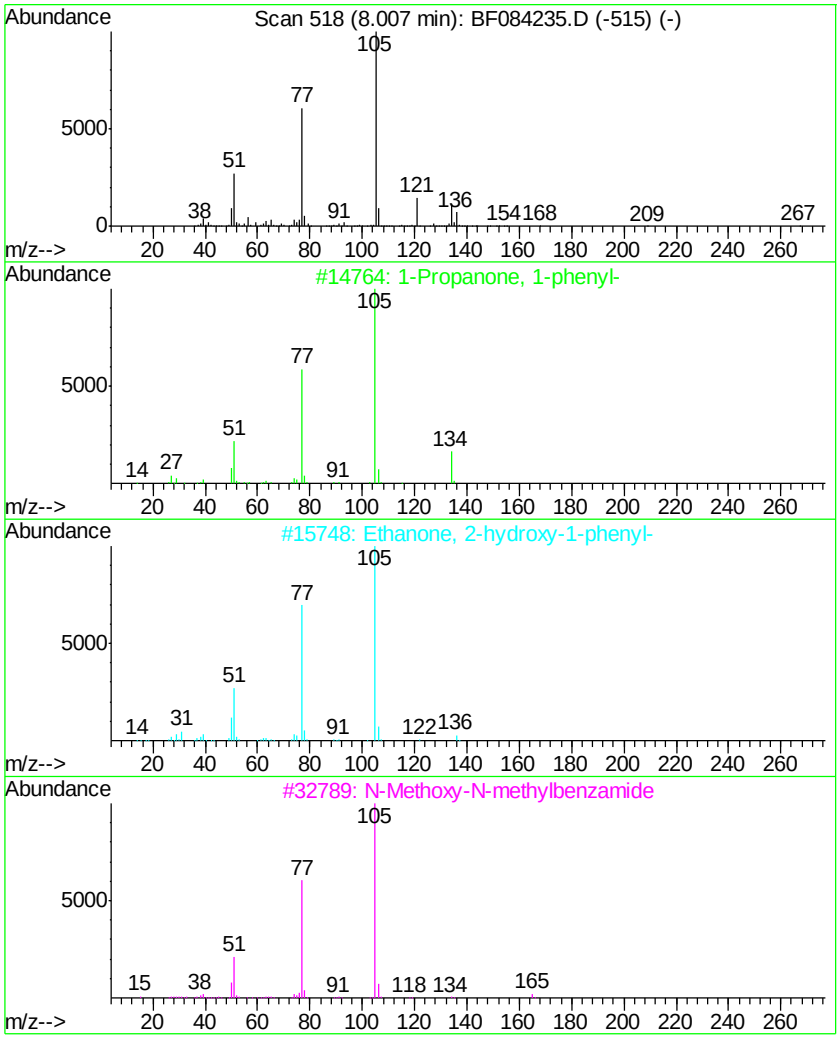
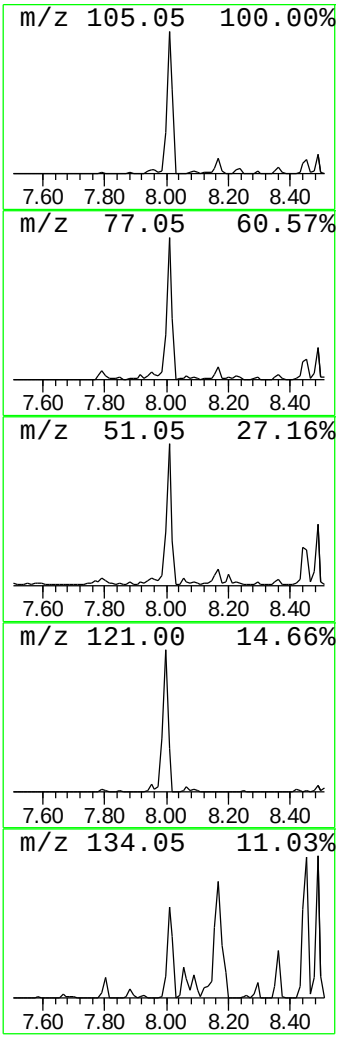
Peak Number 9 1-Propanone, 1-phenyl- Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.01 | 35.51 ng | 13363700 | Naphthalene-d8 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Propanone, 1-phenyl- | 134 | C9H10O | 000093-55-0 | 87 |
| 2 | Ethanone, 2-hydroxy-1-phenyl- | 136 | C8H8O2 | 000582-24-1 | 74 |
| 3 | N-Methoxy-N-methylbenzamide | 165 | C9H11NO2 | 006919-61-5 | 59 |
| 4 | Benzenecarbothioic acid | 138 | C7H6OS | 000098-91-9 | 59 |
| 5 | Benzoic acid, 2-(benzoylthio)thi... | 341 | C17H11NO3S2 | 1000258-72-7 | 59 |



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Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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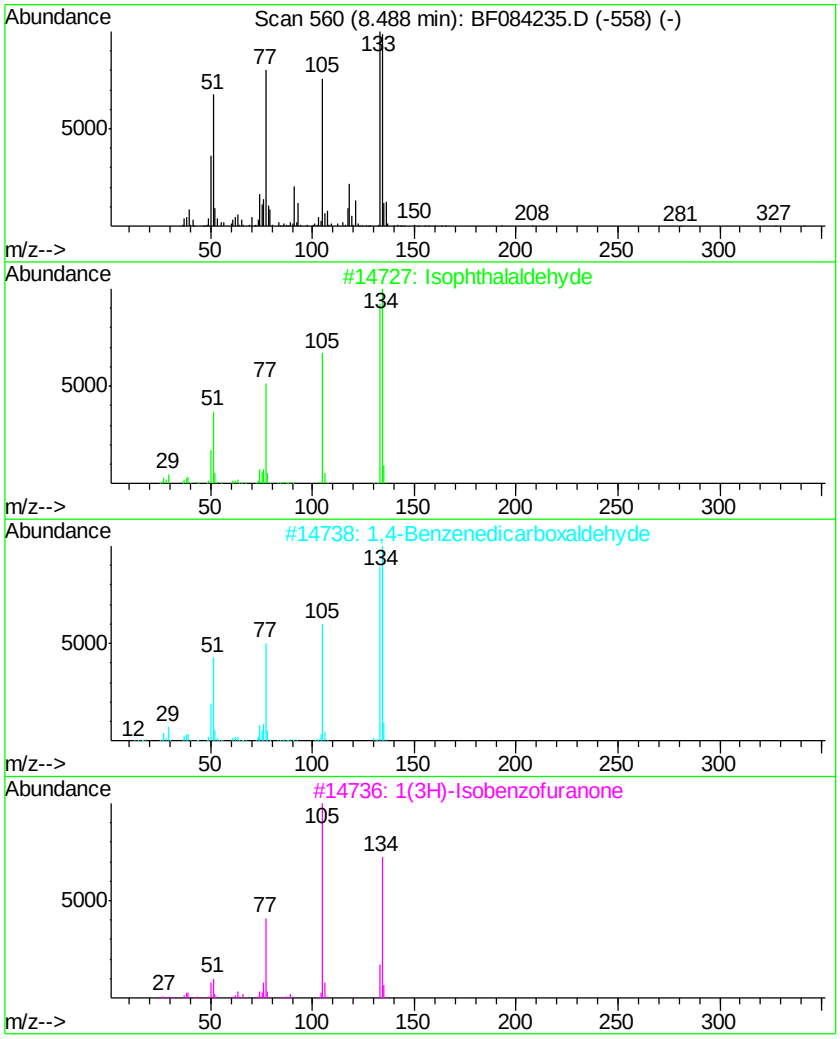
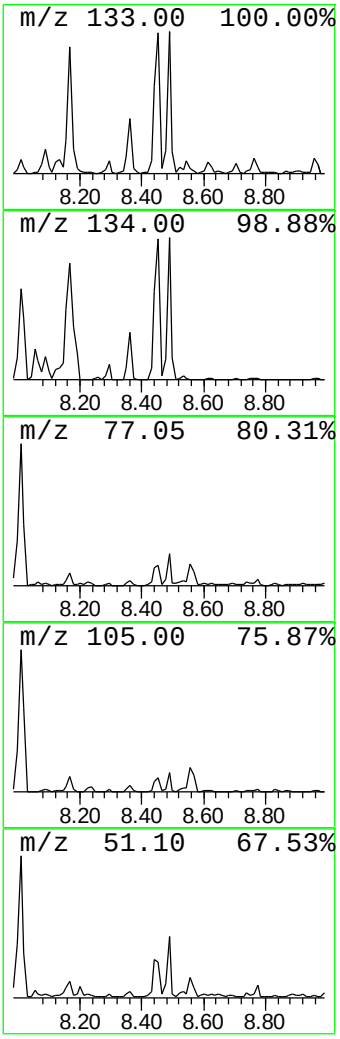
Peak Number 10 Isophthalaldehyde Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.49 | 8.94 ng | 3365110 | Naphthalene-d8 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Isophthalaldehyde | 134 | C8H6O2 | 000626-19-7 | 95 |
| 2 | 1,4-Benzenedicarboxaldehyde | 134 | C8H6O2 | 000623-27-8 | 93 |
| 3 | 1(3H)-Isobenzofuranone | 134 | C8H6O2 | 000087-41-2 | 86 |
| 4 | Benzaldehyde, 2,4-dimethyl- | 134 | C9H10O | 015764-16-6 | 64 |
| 5 | Benzaldehyde, 4-ethyl- | 134 | C9H10O | 004748-78-1 | 47 |



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Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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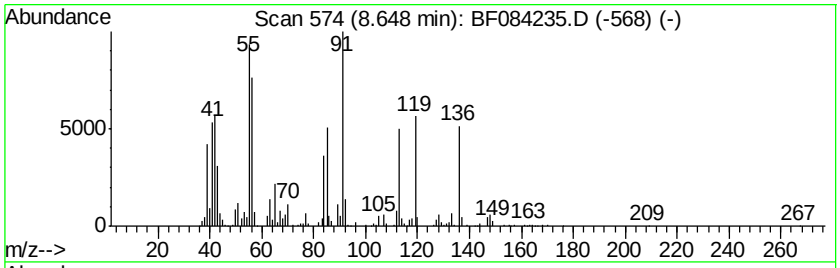
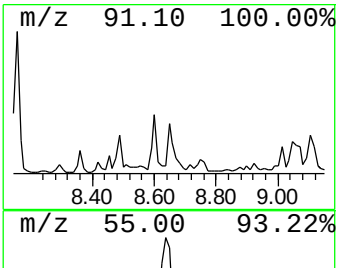
Peak Number 11 Benzoic acid, 4-methyl- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.65 | 11.48 ng | 4321910 | Naphthalene-d8 | 8.18 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 4-methyl- | 136 | C8H8O2 | 000099-94-5 | 91 |
| 2 | Caprolactam | 113 | C6H11NO | 000105-60-2 | 43 |
| 3 | 2H-Pyran-2-one, tetrahydro-3,6-d... | 128 | C7H12O2 | 003720-22-7 | 35 |
| 4 | trans-2,3-Epoxyoctane | 128 | C8H16O | 028180-70-3 | 30 |
| 5 | 1-Pentene, 2-methyl- | 84 | C6H12 | 000763-29-1 | 25 |



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Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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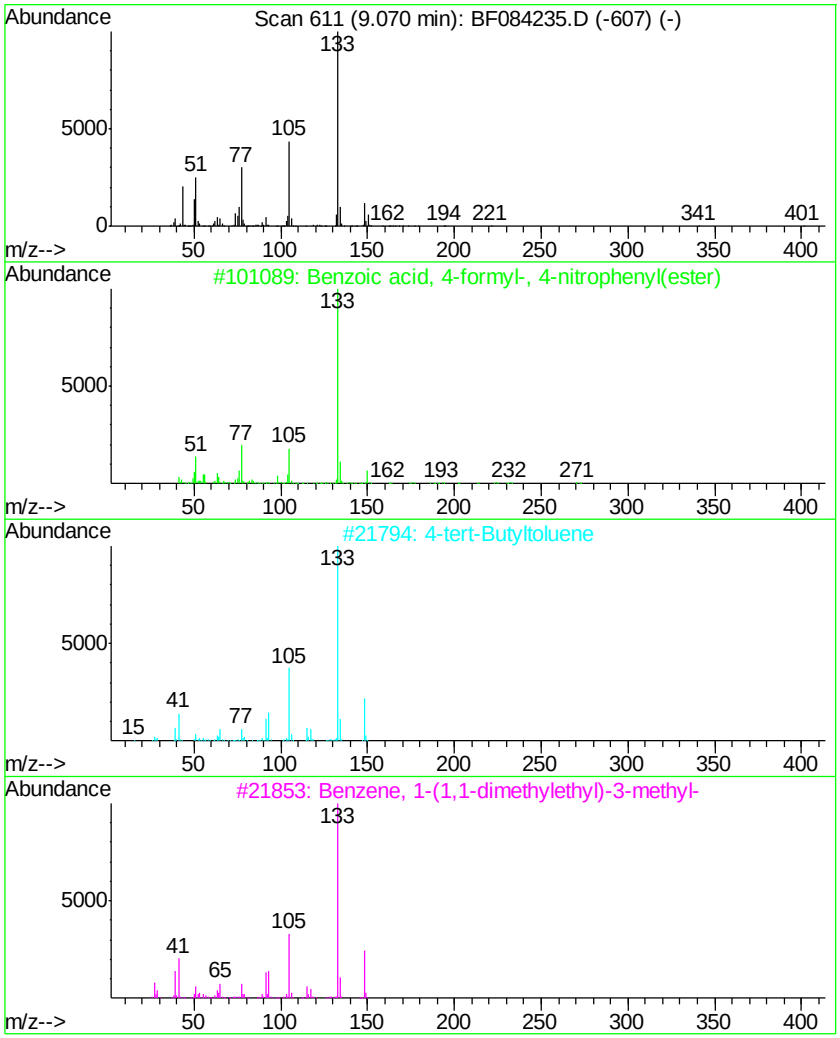
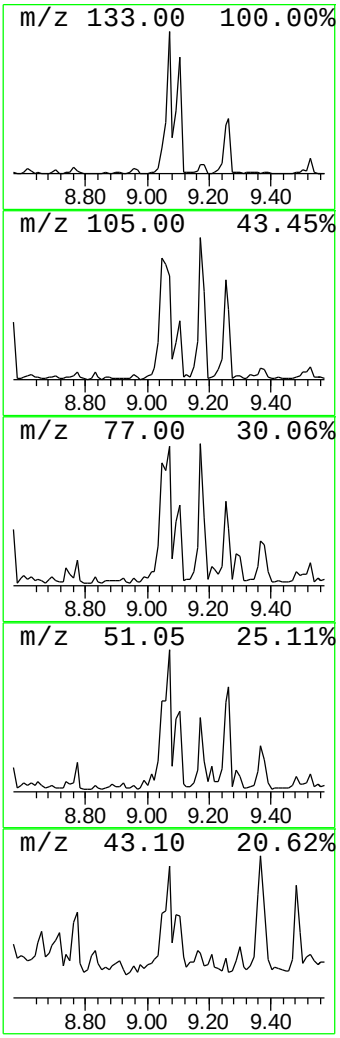
Peak Number 12 Benzoic acid, 4-formyl-, 4-... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.07 | 27.14 ng | 6653600 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 4-formyl-, 4-nitro... | 271 | C14H9NO5 | 131266-90-5 | 78 |
| 2 | 4-tert-Butyltoluene | 148 | C11H16 | 000098-51-1 | 52 |
| 3 | Benzene, 1-(1,1-dimethylethyl)-3... | 148 | C11H16 | 001075-38-3 | 50 |
| 4 | 3,4-Dimethylbenzamide | 149 | C9H11NO | 005580-33-6 | 50 |
| 5 | 1H-Indol-5-ol | 133 | C8H7NO | 001953-54-4 | 50 |



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Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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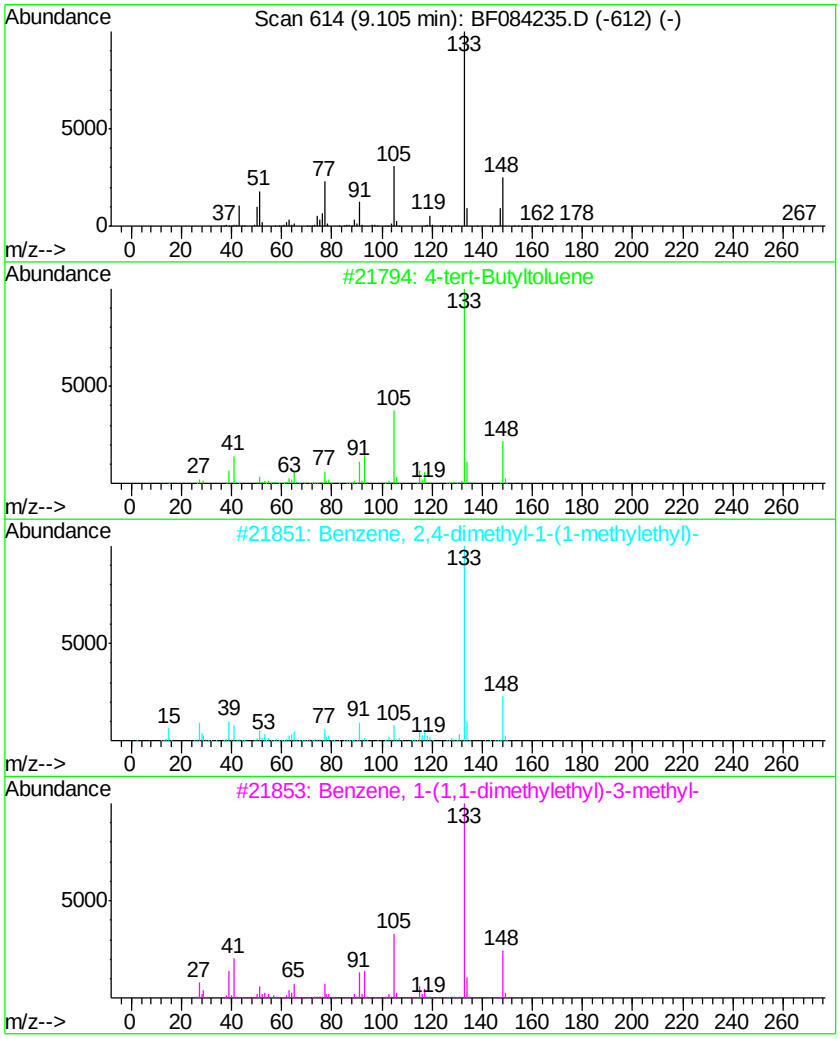
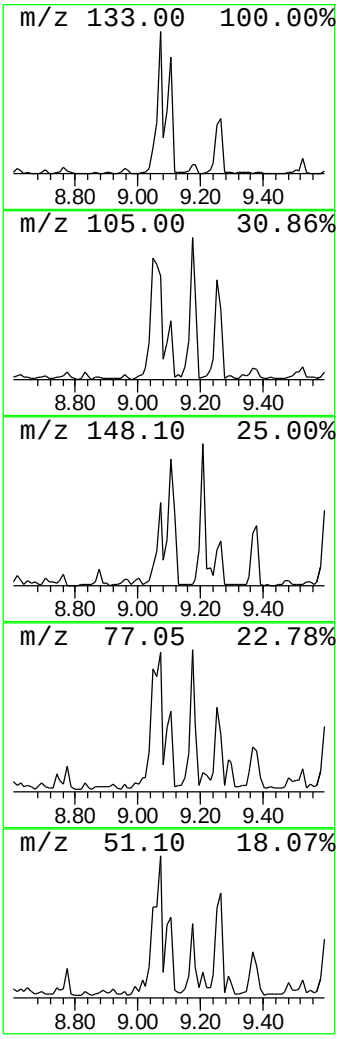
Peak Number 13 4-tert-Butyltoluene Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.10 | 13.55 ng | 3321060 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 4-tert-Butyltoluene | 148 | C11H16 | 000098-51-1 | 64 |
| 2 | Benzene, 2,4-dimethyl-1-(1-methy... | 148 | C11H16 | 004706-89-2 | 64 |
| 3 | Benzene, 1-(1,1-dimethylethyl)-3... | 148 | C11H16 | 001075-38-3 | 64 |
| 4 | Ethanone, 1-(4-ethylphenyl)- | 148 | C10H12O | 000937-30-4 | 64 |
| 5 | 1,5,6,7-Tetramethylbicyclo[3.2.0... | 148 | C11H16 | 134329-46-7 | 59 |



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Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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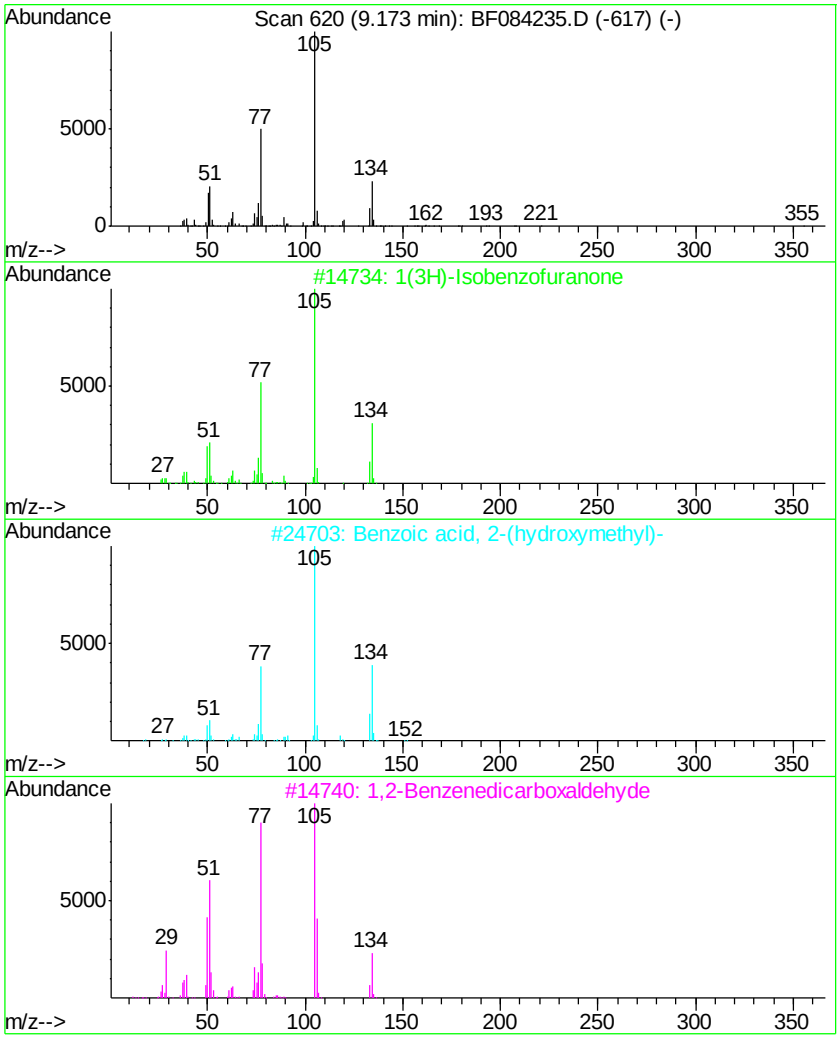
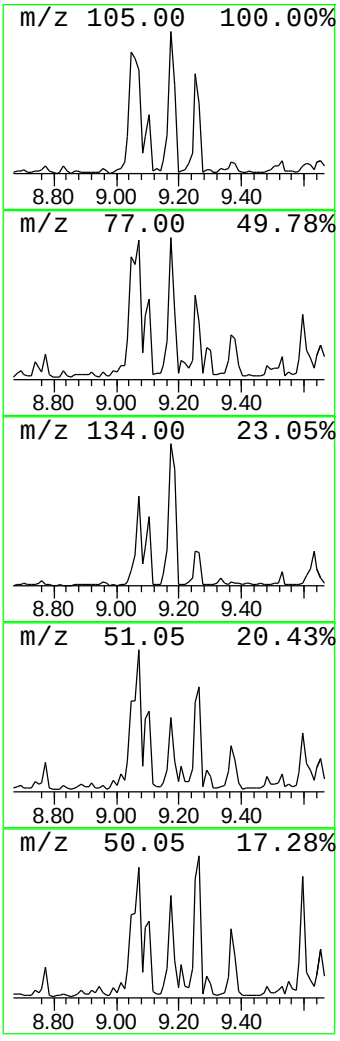
Peak Number 14 1(3H)-Isobenzofuranone Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.17 | 12.85 ng | 3148760 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1(3H)-Isobenzofuranone | 134 | C8H6O2 | 000087-41-2 | 95 |
| 2 | Benzoic acid, 2-(hydroxymethyl)- | 152 | C8H8O3 | 000612-20-4 | 83 |
| 3 | 1,2-Benzenedicarboxaldehyde | 134 | C8H6O2 | 000643-79-8 | 64 |
| 4 | Benzoic acid, (4-nitrophenyl)-me... | 269 | C14H11N3O3 | 028123-77-5 | 53 |
| 5 | Benzofurazan-5-carbohydrazide, N... | 282 | C14H10N4O3 | 1000272-94-4 | 53 |



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Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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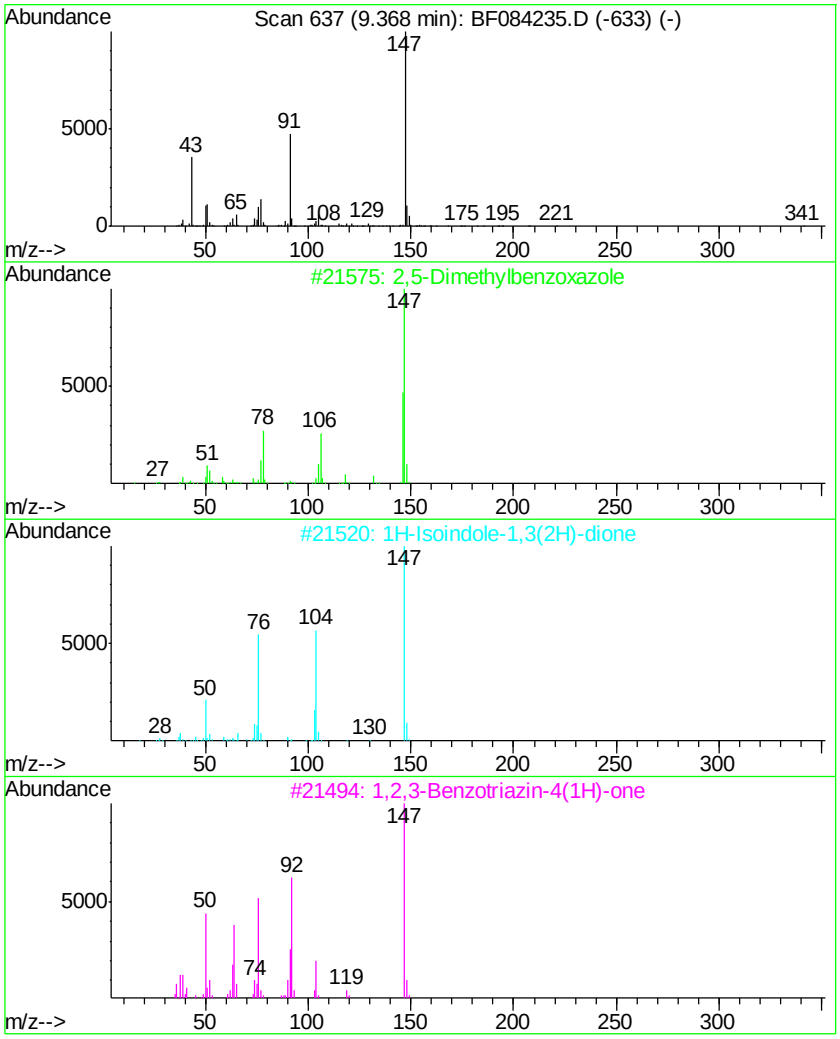
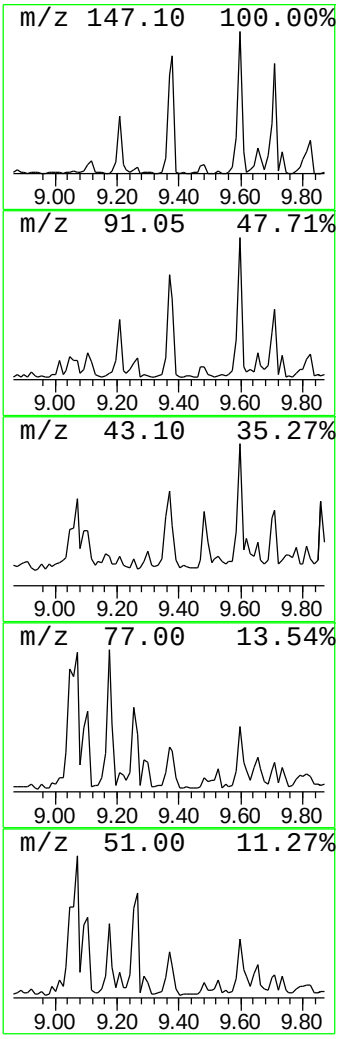
Peak Number 15 2,5-Dimethylbenzoxazole Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.37 | 18.90 ng | 4632920 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2,5-Dimethylbenzoxazole | 147 | C9H9NO | 005676-58-4 | 53 |
| 2 | 1H-Isoindole-1,3(2H)-dione | 147 | C8H5NO2 | 000085-41-6 | 42 |
| 3 | 1,2,3-Benzotriazin-4(1H)-one | 147 | C7H5N3O | 000090-16-4 | 40 |
| 4 | 2H-Indazol-3-amine, 2-methyl- | 147 | C8H9N3 | 097990-19-7 | 33 |
| 5 | Cyclopropanamine, N-methyl-1-phe... | 147 | C10H13N | 056771-48-3 | 33 |



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Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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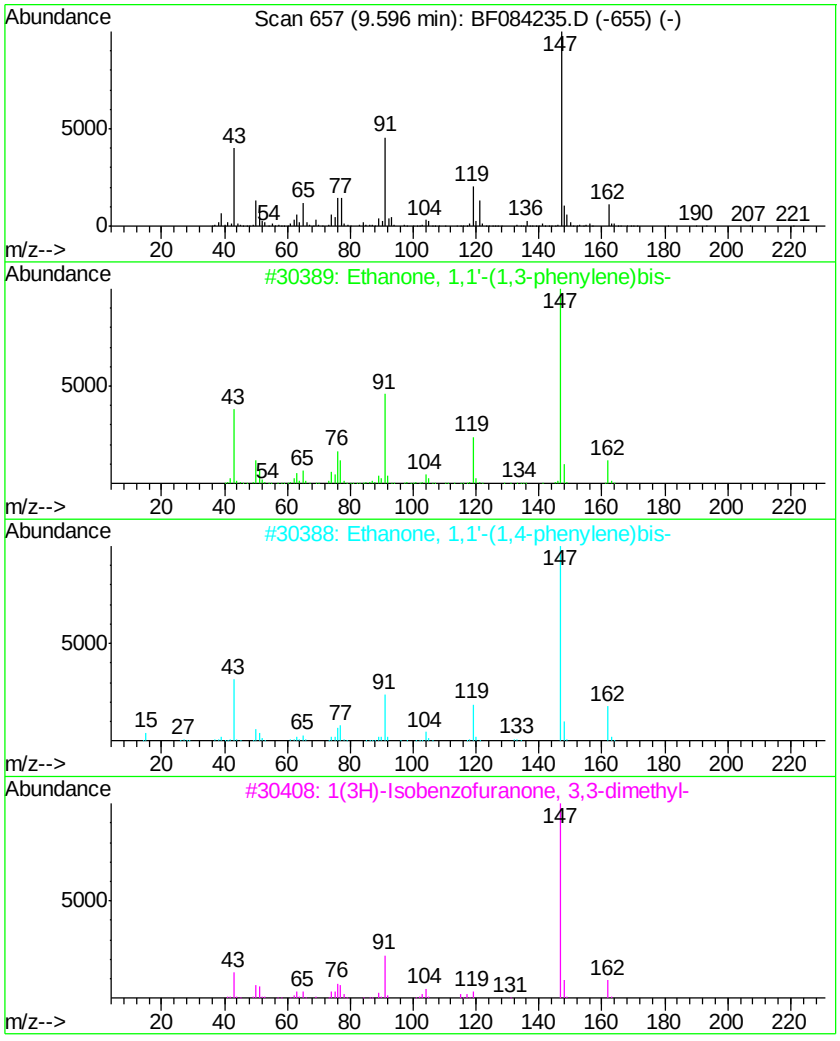
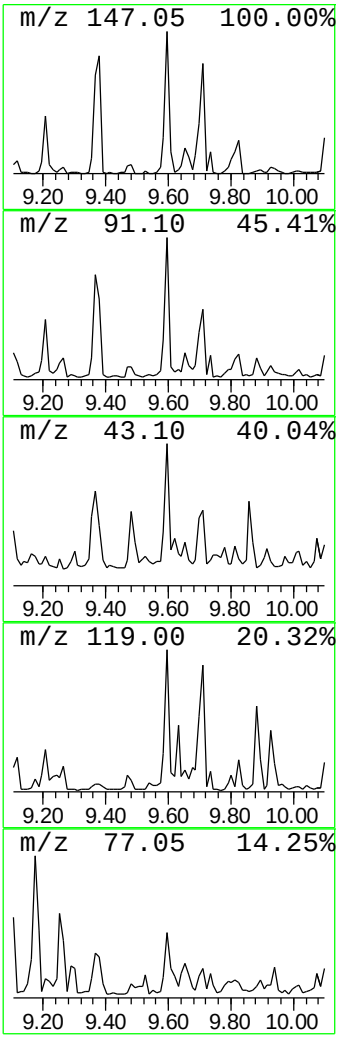
Peak Number 16 Ethanone, 1,1'-(1,3-phenyle... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.60 | 24.48 ng | 6000530 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Ethanone, 1,1'-(1,3-phenylene)bis- | 162 | C10H10O2 | 006781-42-6 | 93 |
| 2 | Ethanone, 1,1'-(1,4-phenylene)bis- | 162 | C10H10O2 | 001009-61-6 | 93 |
| 3 | 1(3H)-Isobenzofuranone, 3,3-dime... | 162 | C10H10O2 | 001689-09-4 | 64 |
| 4 | Pyrido[2,3-d]pyrimidin-4(1H)-one | 147 | C7H5N3O | 024410-19-3 | 59 |
| 5 | o-Diacetylbenzene | 162 | C10H10O2 | 000704-00-7 | 58 |



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Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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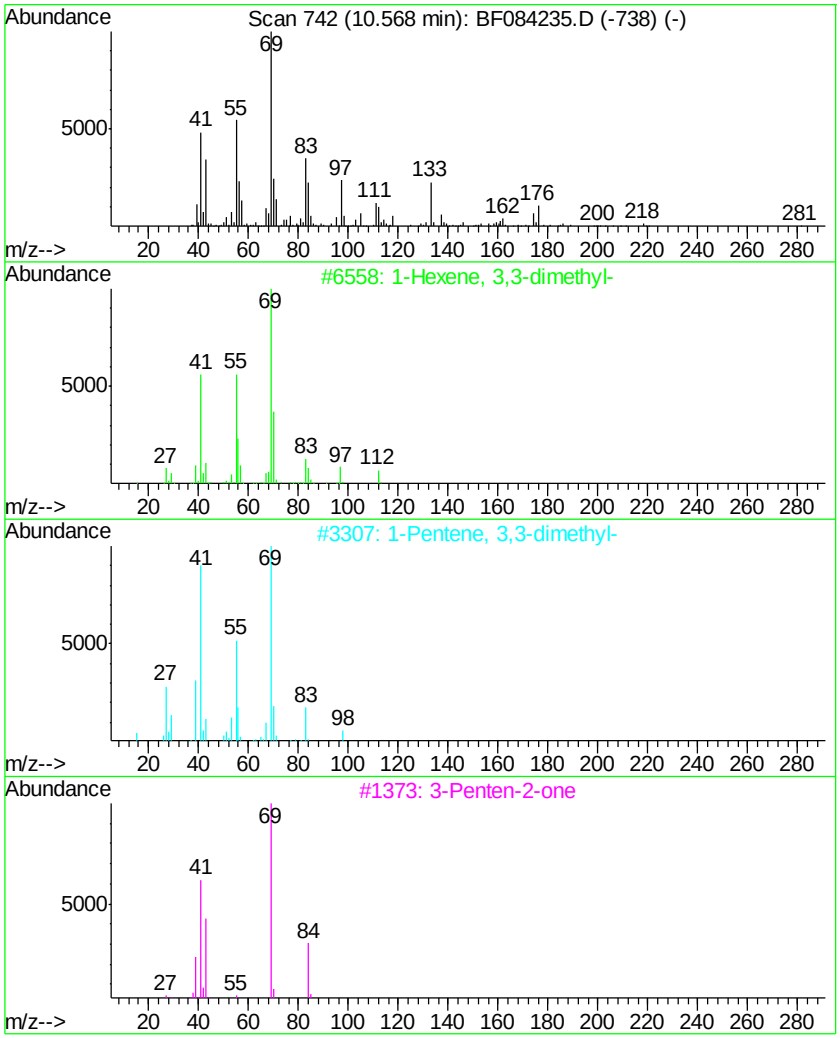
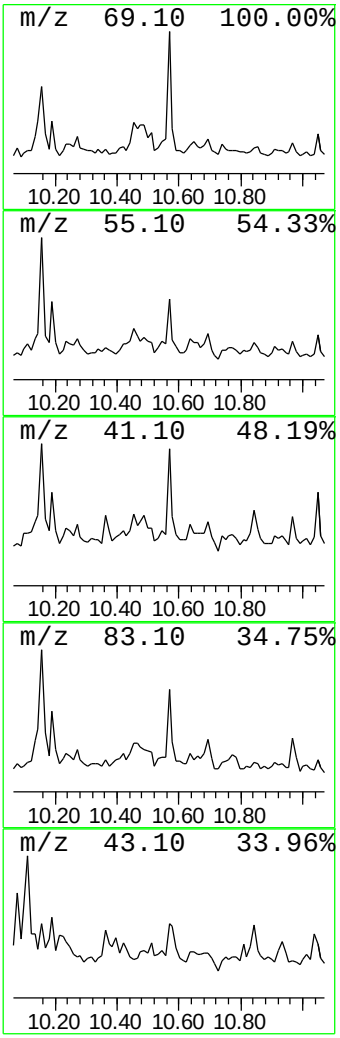
Peak Number 17 unknown10.57 Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.57 | 8.86 ng | 2171390 | Acenaphthene-d10 | 9.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Hexene, 3,3-dimethyl- | 112 | C8H16 | 003404-77-1 | 49 |
| 2 | 1-Pentene, 3,3-dimethyl- | 98 | C7H14 | 003404-73-7 | 38 |
| 3 | 3-Penten-2-one | 84 | C5H8O | 000625-33-2 | 38 |
| 4 | Cyclohexane, 1-ethyl-1,4-dimethy... | 140 | C10H20 | 062238-32-8 | 38 |
| 5 | 1-Butene, 3,3-dimethyl- | 84 | C6H12 | 000558-37-2 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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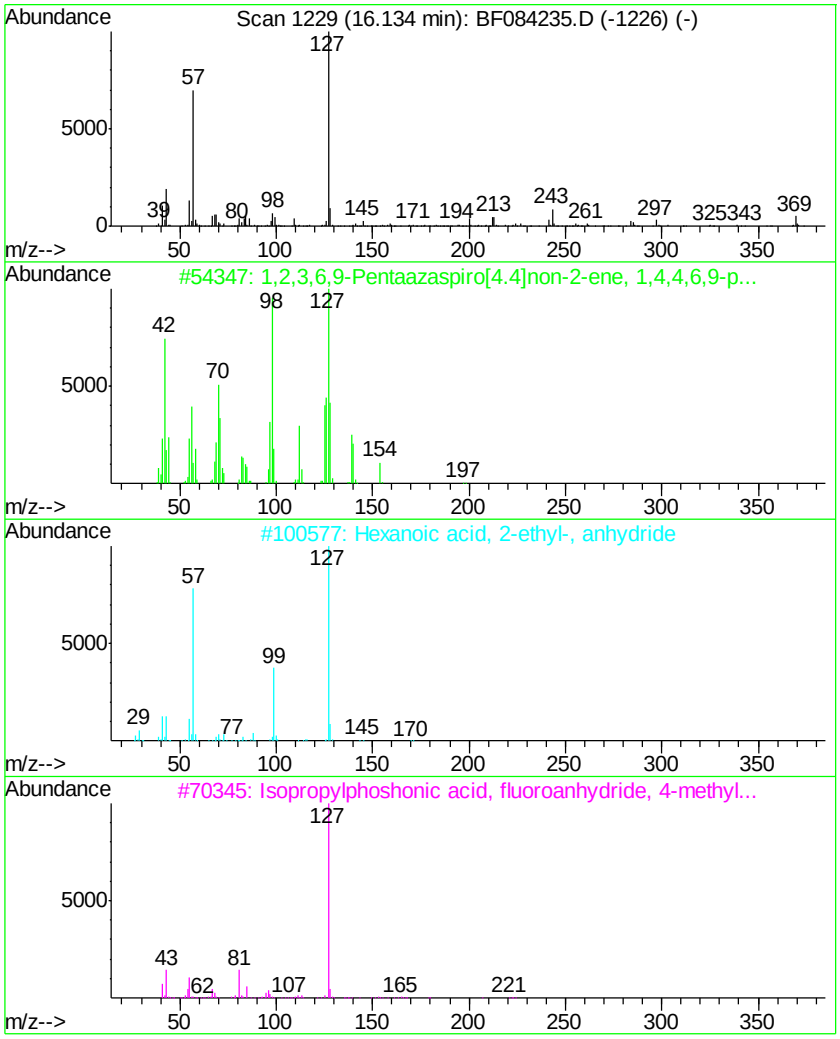
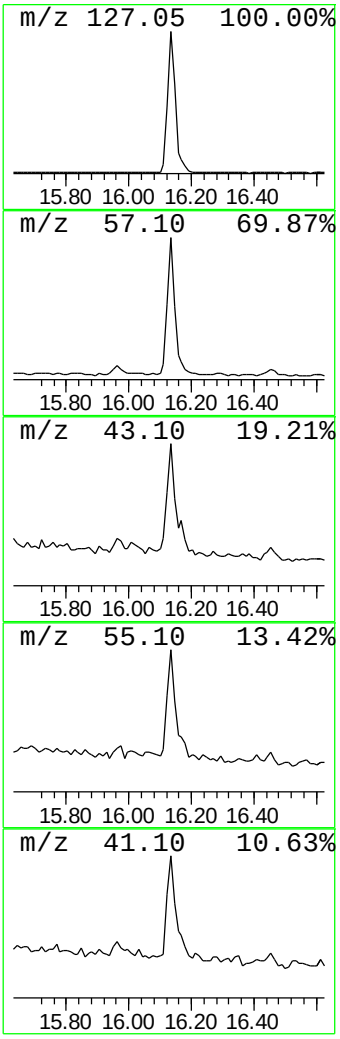
Peak Number 18 1,2,3,6,9-Pentaazaspiro[4.4... Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 16.13 | 19.99 ng | 1131270 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,2,3,6,9-Pentaazaspiro[4.4]non-... | 197 | C9H19N5 | 1000221-38-7 | 64 |
| 2 | Hexanoic acid, 2-ethyl-, anhydride | 270 | C16H30O3 | 036765-89-6 | 59 |
| 3 | Isopropylphoshonic acid, fluoroa... | 222 | C10H20FO2P | 1000273-48-8 | 59 |
| 4 | 1H-Imidazole, 1-methyl-4-nitro- | 127 | C4H5N3O2 | 003034-41-1 | 53 |
| 5 | Spiro[bicyclo[2.2.1]heptane-2,2'... | 212 | C12H20O3 | 035972-92-0 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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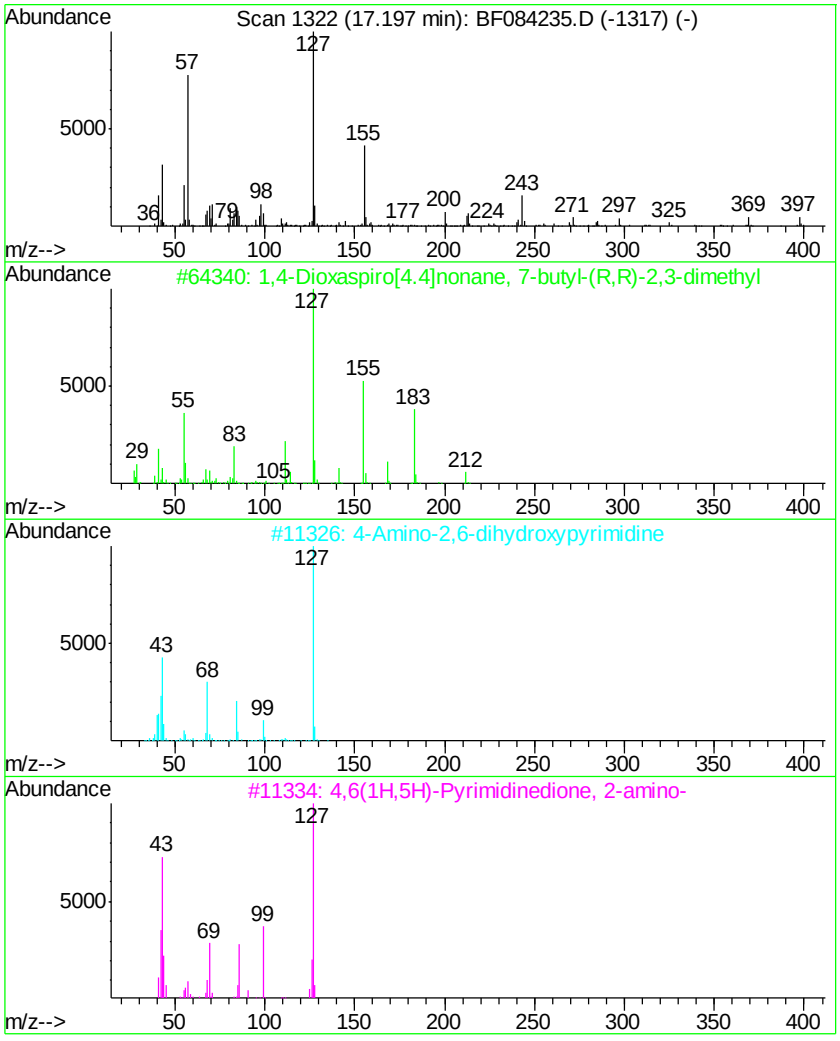
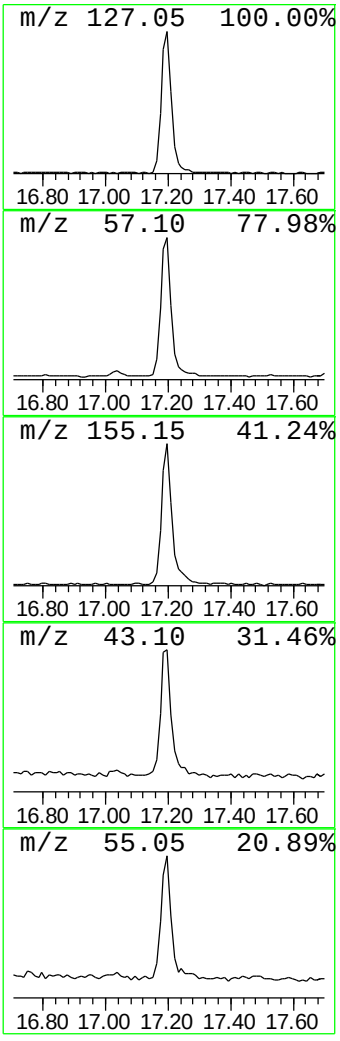
Peak Number 19 1,4-Dioxaspiro[4.4]nonane, ... Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 17.20 | 31.23 ng | 1767580 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Dioxaspiro[4.4]nonane, 7-but... | 212 | C13H24O2 | 104807-77-4 | 72 |
| 2 | 4-Amino-2,6-dihydroxypyrimidine | 127 | C4H5N3O2 | 000873-83-6 | 43 |
| 3 | 4,6(1H,5H)-Pyrimidinedione, 2-am... | 127 | C4H5N3O2 | 004425-67-6 | 38 |
| 4 | 2-Butenedioic acid (E)-, diethyl... | 172 | C8H12O4 | 000623-91-6 | 38 |
| 5 | 2-Amino-4,6-dihydroxypyrimidine | 127 | C4H5N3O2 | 000056-09-7 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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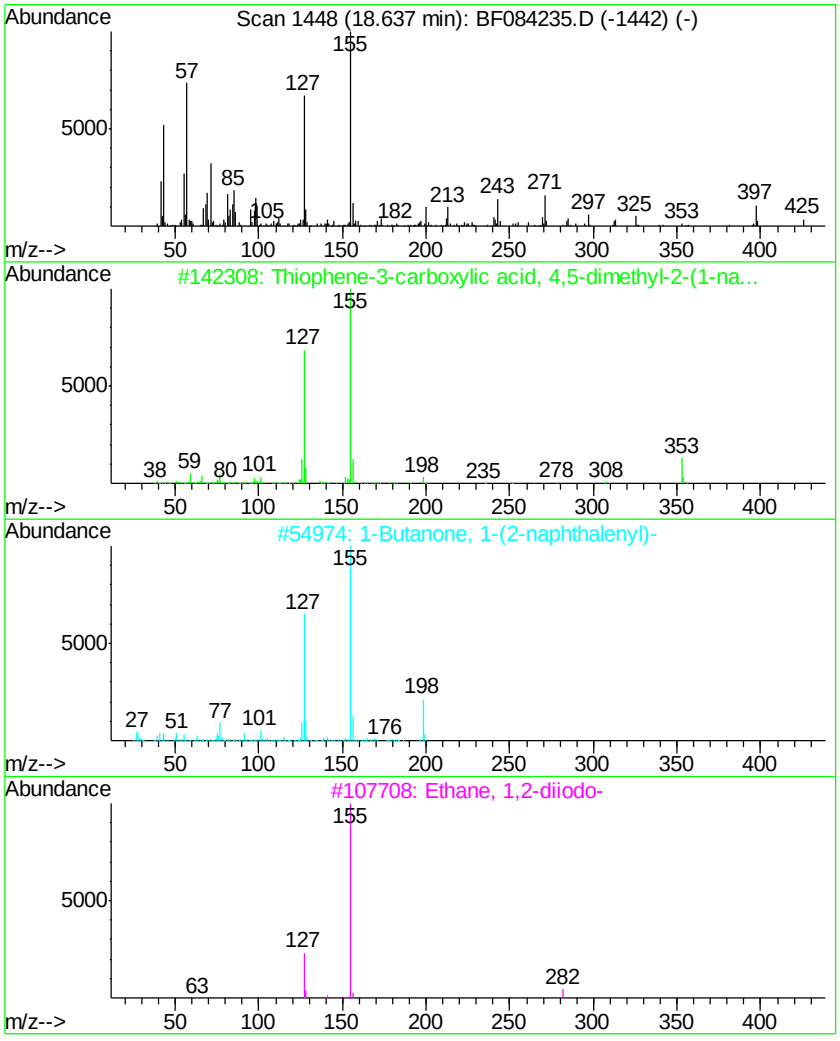
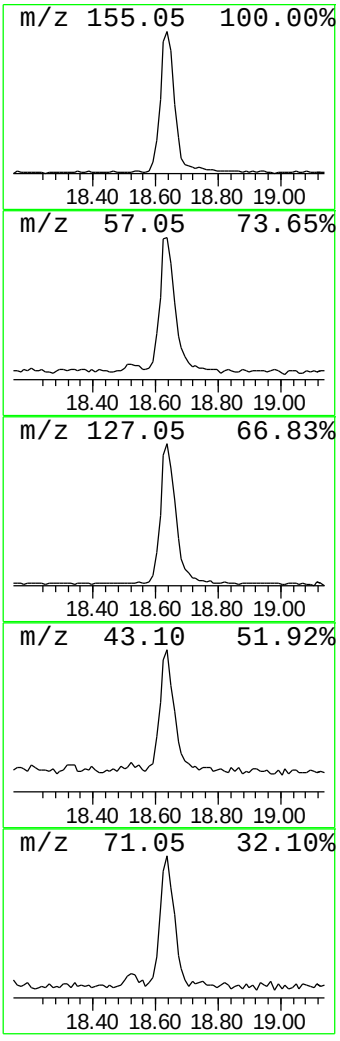
Peak Number 20 Thiophene-3-carboxylic acid... Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.64 | 20.82 ng | 1178470 | Perylene-d12 | 15.49 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Thiophene-3-carboxylic acid, 4,5... | 353 | C20H19NO3S | 327049-67-2 | 53 |
| 2 | 1-Butanone, 1-(2-naphthalenyl)- | 198 | C14H14O | 017666-88-5 | 53 |
| 3 | Ethane, 1,2-diiodo- | 282 | C2H4I2 | 000624-73-7 | 53 |
| 4 | 5-Oxazolidinone, 2-(1,1-dimethyl... | 297 | C18H19NO3 | 119215-55-3 | 52 |
| 5 | 5-Oxazolidinone, 2-(1,1-dimethyl... | 297 | C18H19NO3 | 119215-56-4 | 52 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF010416\
Data File : BF084235.D
Acq On : 4 Jan 2016 13:32
Operator : UM/SJ
Sample : G4982-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** S8-0530

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF123115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| unknown5.08 | 5.08 | 10.3 | ng | 2520830 | 1 | 6.89 | 4911200 | 20.0 |
| Ethane, 1,1,2,2-t... | 6.02 | 12.5 | ng | 3076700 | 1 | 6.89 | 4911200 | 20.0 |
| 2,3,3-Trimethyl-2... | 6.10 | 12.4 | ng | 3037320 | 1 | 6.89 | 4911200 | 20.0 |
| unknown6.67 | 6.67 | 37.4 | ng | 9190520 | 1 | 6.89 | 4911200 | 20.0 |
| 1-Methyl-1H-1,2,4... | 6.97 | 11.0 | ng | 2707810 | 1 | 6.89 | 4911200 | 20.0 |
| unknown7.60 | 7.60 | 12.3 | ng | 4609840 | 2 | 8.18 | 7527040 | 20.0 |
| unknown7.77 | 7.77 | 23.6 | ng | 8874010 | 2 | 8.18 | 7527040 | 20.0 |
| 1-Propanone, 1-ph... | 8.01 | 35.5 | ng | 13363700 | 2 | 8.18 | 7527040 | 20.0 |
| Isophthalaldehyde | 8.49 | 8.9 | ng | 3365110 | 2 | 8.18 | 7527040 | 20.0 |
| Benzoic acid, 4-m... | 8.65 | 11.5 | ng | 4321910 | 2 | 8.18 | 7527040 | 20.0 |
| Benzoic acid, 4-f... | 9.07 | 27.1 | ng | 6653600 | 3 | 9.94 | 4902310 | 20.0 |
| 4-tert-Butyltoluene | 9.10 | 13.6 | ng | 3321060 | 3 | 9.94 | 4902310 | 20.0 |
| 1(3H)-Isobenzofur... | 9.17 | 12.9 | ng | 3148760 | 3 | 9.94 | 4902310 | 20.0 |
| 2,5-Dimethylbenzo... | 9.37 | 18.9 | ng | 4632920 | 3 | 9.94 | 4902310 | 20.0 |
| Ethanone, 1,1'-(1... | 9.60 | 24.5 | ng | 6000530 | 3 | 9.94 | 4902310 | 20.0 |
| unknown10.57 | 10.57 | 8.9 | ng | 2171390 | 3 | 9.94 | 4902310 | 20.0 |
| 1,2,3,6,9-Pentaaz... | 16.13 | 20.0 | ng | 1131270 | 6 | 15.49 | 1131920 | 20.0 |
| 1,4-Dioxaspiro[4.... | 17.20 | 31.2 | ng | 1767580 | 6 | 15.49 | 1131920 | 20.0 |
| Thiophene-3-carbo... | 18.64 | 20.8 | ng | 1178470 | 6 | 15.49 | 1131920 | 20.0 |