LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

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-BF101116.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 | 5.137 | 243 | 245 | 261 | rBV | 256254 | 371671 | 5.27% | 0.657% |
| 2 | 5.560 | 280 | 282 | 301 | rBV | 703610 | 1651819 | 23.42% | 2.918% |
| 3 | 6.543 | 366 | 368 | 370 | rBV | 193537 | 183219 | 2.60% | 0.324% |
| 4 | 6.589 | 370 | 372 | 381 | rVB | 542316 | 1123507 | 15.93% | 1.985% |
| 5 | 6.714 | 381 | 383 | 398 | rVB | 2560362 | 3332823 | 47.26% | 5.888% |
| 6 | 6.943 | 401 | 403 | 407 | rBV | 891788 | 1166808 | 16.55% | 2.061% |
| 7 | 7.103 | 415 | 417 | 424 | rBV | 4325408 | 4445272 | 63.04% | 7.853% |
| 8 | 7.194 | 424 | 425 | 429 | rVB | 67060 | 80671 | 1.14% | 0.143% |
| 9 | 7.263 | 429 | 431 | 433 | rBV | 250899 | 272206 | 3.86% | 0.481% |
| 10 | 7.297 | 433 | 434 | 437 | rVB | 194718 | 216757 | 3.07% | 0.383% |
| 11 | 7.515 | 450 | 453 | 455 | rBV | 2869974 | 3528156 | 50.03% | 6.233% |
| 12 | 7.743 | 471 | 473 | 477 | rVB | 178897 | 171082 | 2.43% | 0.302% |
| 13 | 7.857 | 479 | 483 | 484 | rVV | 82218 | 132658 | 1.88% | 0.234% |
| 14 | 7.892 | 484 | 486 | 491 | rVV2 | 204057 | 320922 | 4.55% | 0.567% |
| 15 | 7.972 | 491 | 493 | 495 | rVV | 105279 | 131690 | 1.87% | 0.233% |
| 16 | 8.029 | 495 | 498 | 503 | rVB2 | 94251 | 189659 | 2.69% | 0.335% |
| 17 | 8.235 | 513 | 516 | 521 | rVB | 1506491 | 1704104 | 24.17% | 3.011% |
| 18 | 8.315 | 521 | 523 | 526 | rVB2 | 63859 | 94039 | 1.33% | 0.166% |
| 19 | 8.395 | 528 | 530 | 535 | rBV2 | 301710 | 500214 | 7.09% | 0.884% |
| 20 | 8.497 | 535 | 539 | 541 | rBV | 967893 | 1171399 | 16.61% | 2.069% |
| 21 | 8.532 | 541 | 542 | 546 | rVB | 352294 | 465324 | 6.60% | 0.822% |
| 22 | 8.623 | 548 | 550 | 552 | rBV2 | 68812 | 79770 | 1.13% | 0.141% |
| 23 | 8.703 | 556 | 557 | 559 | rBV | 65806 | 85787 | 1.22% | 0.152% |
| 24 | 8.738 | 559 | 560 | 563 | rVB | 136798 | 143364 | 2.03% | 0.253% |
| 25 | 8.795 | 563 | 565 | 566 | rBV | 59091 | 82930 | 1.18% | 0.147% |
| 26 | 8.829 | 566 | 568 | 570 | rBV | 491430 | 579852 | 8.22% | 1.024% |
| 27 | 8.955 | 576 | 579 | 582 | rBV | 109367 | 189394 | 2.69% | 0.335% |
| 28 | 9.012 | 582 | 584 | 585 | rVV2 | 76506 | 123849 | 1.76% | 0.219% |
| 29 | 9.035 | 585 | 586 | 588 | rVV2 | 154194 | 262768 | 3.73% | 0.464% |
| 30 | 9.069 | 588 | 589 | 592 | rVV2 | 153903 | 261853 | 3.71% | 0.463% |
| 31 | 9.126 | 592 | 594 | 598 | rVB2 | 97778 | 179132 | 2.54% | 0.316% |
| 32 | 9.275 | 605 | 607 | 608 | rBV | 53999 | 83073 | 1.18% | 0.147% |
| 33 | 9.309 | 608 | 610 | 613 | rVB | 5295310 | 6680741 | 94.74% | 11.803% |
| 34 | 9.480 | 621 | 625 | 626 | rBV3 | 55909 | 94511 | 1.34% | 0.167% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

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-BF101116.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.560 | 629 | 632 | 637 | rVV4 | 156097 | 524481 | 7.44% | 0.927% |
| 36 | 9.640 | 637 | 639 | 643 | rVB2 | 71715 | 147741 | 2.10% | 0.261% |
| 37 | 9.709 | 643 | 645 | 648 | rBV2 | 73065 | 149648 | 2.12% | 0.264% |
| 38 | 9.766 | 648 | 650 | 652 | rVB | 250113 | 230583 | 3.27% | 0.407% |
| 39 | 9.926 | 662 | 664 | 666 | rBV2 | 59671 | 86823 | 1.23% | 0.153% |
| 40 | 9.995 | 667 | 670 | 671 | rBV | 1841008 | 2079241 | 29.49% | 3.673% |
| 41 | 10.029 | 671 | 673 | 675 | rVV | 1801272 | 2114956 | 29.99% | 3.736% |
| 42 | 10.098 | 676 | 679 | 681 | rBV2 | 166223 | 229776 | 3.26% | 0.406% |
| 43 | 10.235 | 690 | 691 | 695 | rVB | 76368 | 86876 | 1.23% | 0.153% |
| 44 | 10.303 | 695 | 697 | 700 | rBV | 116073 | 166471 | 2.36% | 0.294% |
| 45 | 10.475 | 708 | 712 | 717 | rBV | 606409 | 940033 | 13.33% | 1.661% |
| 46 | 10.589 | 720 | 722 | 726 | rBV2 | 162163 | 382612 | 5.43% | 0.676% |
| 47 | 10.646 | 726 | 727 | 730 | rVB | 95113 | 115706 | 1.64% | 0.204% |
| 48 | 10.783 | 736 | 739 | 745 | rVB | 3087991 | 3268573 | 46.35% | 5.774% |
| 49 | 10.909 | 747 | 750 | 752 | rBV | 1226133 | 1668673 | 23.66% | 2.948% |
| 50 | 10.943 | 752 | 753 | 755 | rVB2 | 79013 | 73329 | 1.04% | 0.130% |
| 51 | 11.001 | 755 | 758 | 759 | rBV3 | 67082 | 119486 | 1.69% | 0.211% |
| 52 | 11.149 | 769 | 771 | 776 | rVB4 | 80747 | 170995 | 2.42% | 0.302% |
| 53 | 11.263 | 779 | 781 | 785 | rBV | 191589 | 242220 | 3.43% | 0.428% |
| 54 | 11.435 | 794 | 796 | 798 | rBV2 | 48889 | 76318 | 1.08% | 0.135% |
| 55 | 11.481 | 798 | 800 | 802 | rVV | 2102705 | 1913179 | 27.13% | 3.380% |
| 56 | 11.538 | 802 | 805 | 808 | rVB3 | 48444 | 104064 | 1.48% | 0.184% |
| 57 | 11.595 | 808 | 810 | 813 | rBV3 | 48004 | 77287 | 1.10% | 0.137% |
| 58 | 11.698 | 816 | 819 | 823 | rBV5 | 29387 | 78104 | 1.11% | 0.138% |
| 59 | 11.766 | 823 | 825 | 827 | rVB | 79827 | 83949 | 1.19% | 0.148% |
| 60 | 11.858 | 832 | 833 | 838 | rVB4 | 49654 | 82489 | 1.17% | 0.146% |
| 61 | 12.006 | 844 | 846 | 848 | rBV2 | 56802 | 74818 | 1.06% | 0.132% |
| 62 | 12.098 | 852 | 854 | 855 | rVB | 96807 | 117073 | 1.66% | 0.207% |
| 63 | 12.692 | 903 | 906 | 908 | rVB | 191906 | 171938 | 2.44% | 0.304% |
| 64 | 12.738 | 908 | 910 | 913 | rBV2 | 55471 | 81975 | 1.16% | 0.145% |
| 65 | 12.921 | 924 | 926 | 928 | rBV | 331520 | 291704 | 4.14% | 0.515% |
| 66 | 13.069 | 936 | 939 | 942 | rBV | 7141268 | 7051806 | 100.00% | 12.458% |
| 67 | 13.961 | 1015 | 1017 | 1021 | rBV | 97226 | 115503 | 1.64% | 0.204% |
| 68 | 14.121 | 1028 | 1031 | 1033 | rBV | 2125533 | 1919623 | 27.22% | 3.391% |
| 69 | 15.595 | 1157 | 1160 | 1163 | rBV | 1144075 | 1464976 | 20.77% | 2.588% |

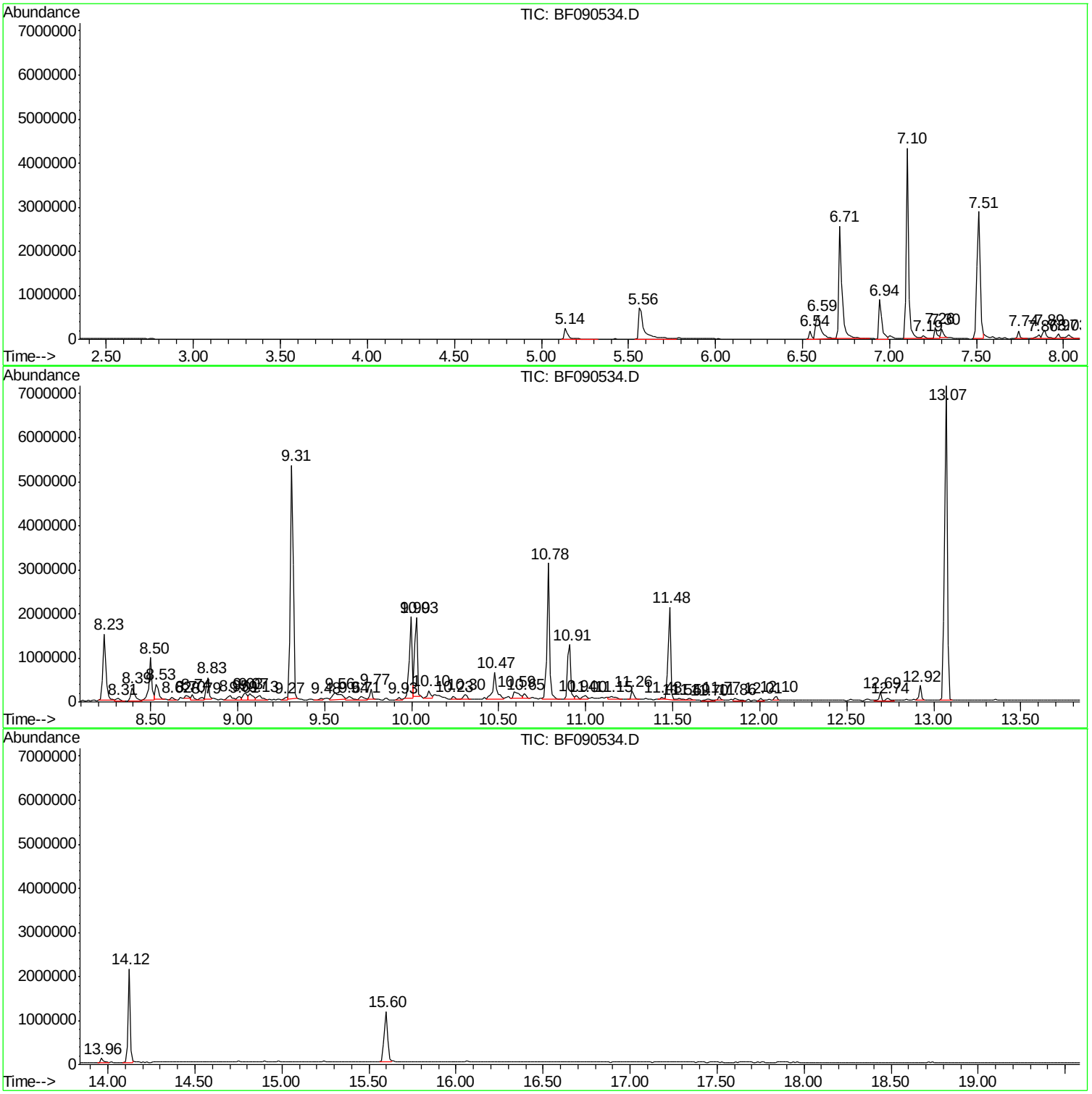
Sum of corrected areas: 56604053

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

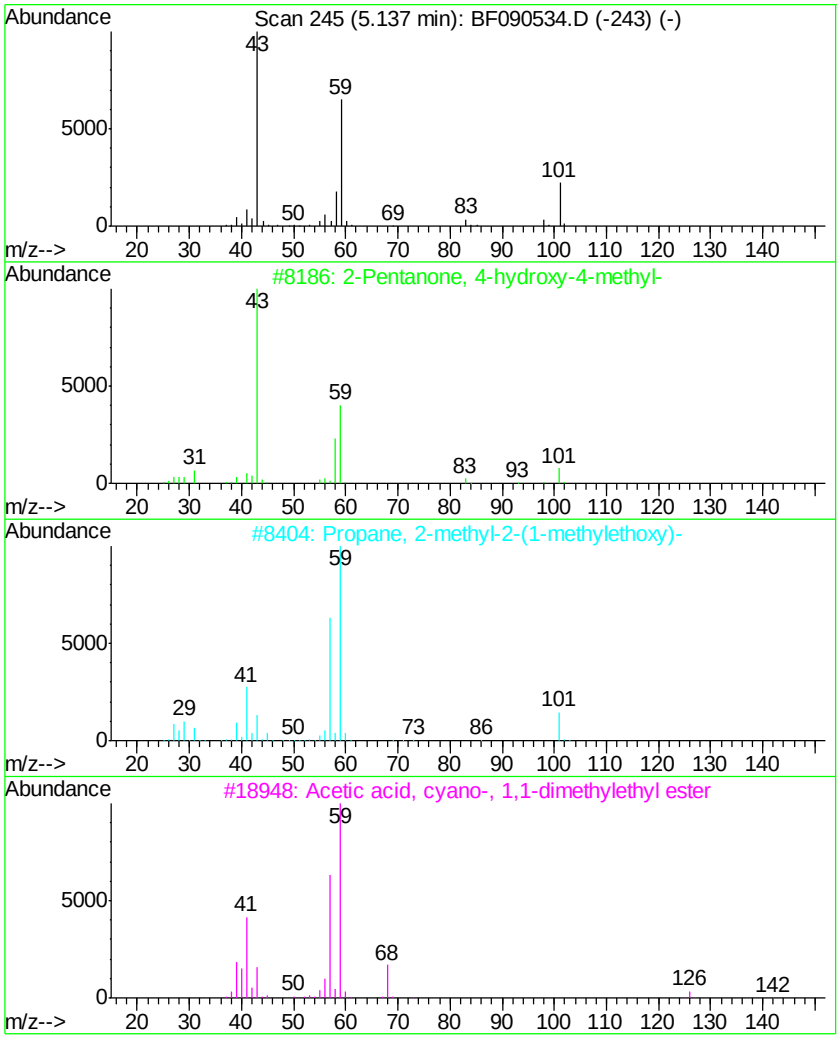
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

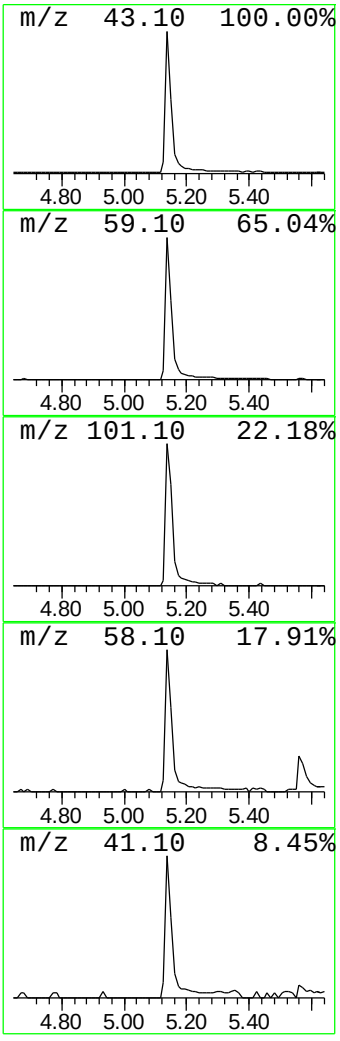
**********

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 5.14 | 6.37 ng | 371671 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Propane, 2-methyl-2-(1-methyleth... | 116 | C7H16O | 017348-59-3 | 40 |
| 3 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 4 | Acetone | 58 | C3H6O | 000067-64-1 | 9 |
| 5 | Guanidine | 59 | CH5N3 | 000113-00-8 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

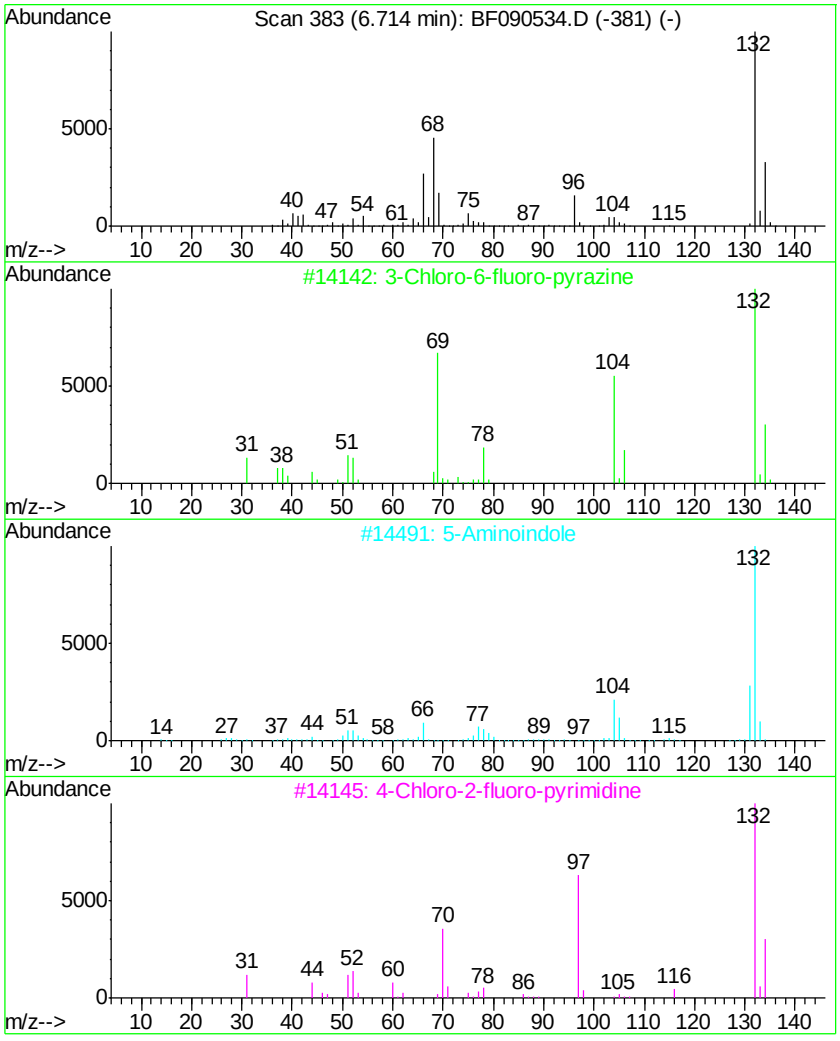
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

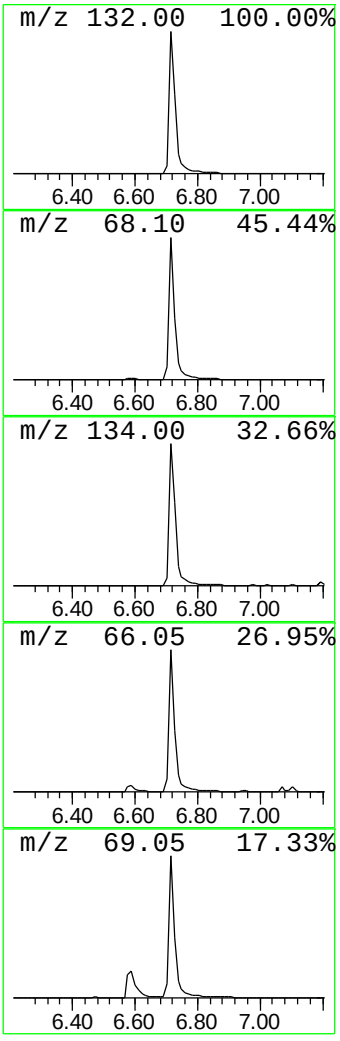
**********

Peak Number 2 unknown6.71 Concentration Rank 2

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.71 | 57.13 ng | 3332820 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 16 |
| 2 | 5-Aminoindole | 132 | C8H8N2 | 005192-03-0 | 12 |
| 3 | 4-Chloro-2-fluoro-pyrimidine | 132 | C4H2ClFN2 | 051422-00-5 | 9 |
| 4 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |
| 5 | 4-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-60-2 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

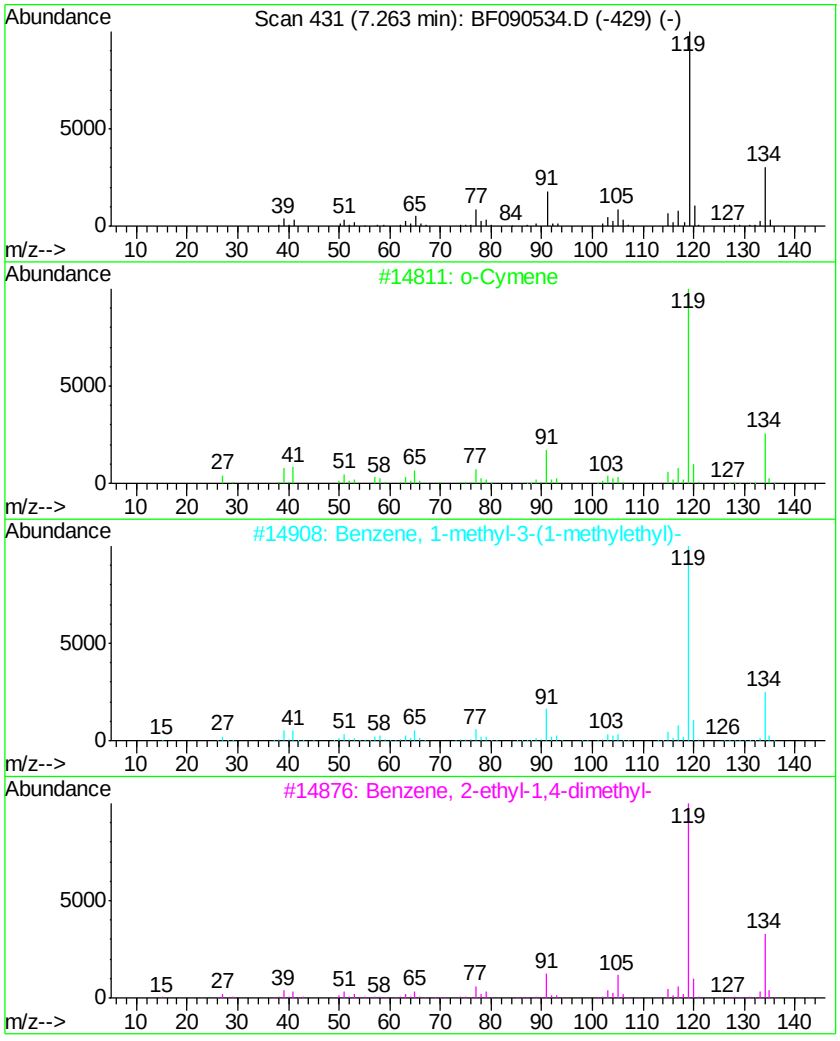
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

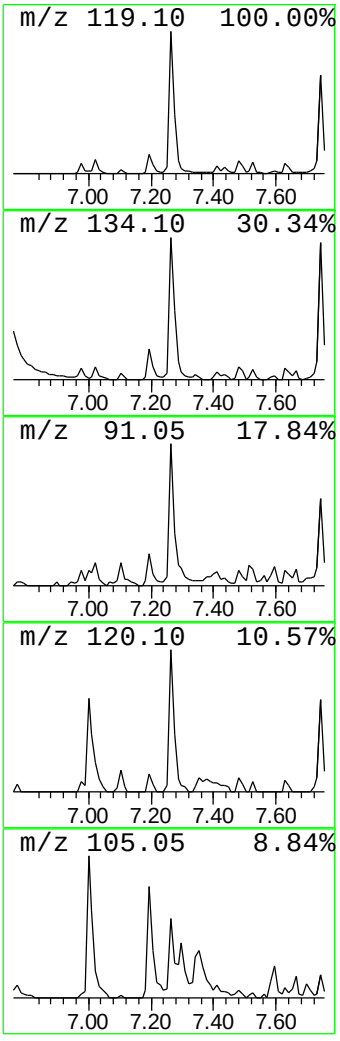
**********

Peak Number 4 o-Cymene Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.26 | 4.67 ng | 272206 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | o-Cymene | 134 | C10H14 | 000527-84-4 | 97 |
| 2 | Benzene, 1-methyl-3-(1-methyleth... | 134 | C10H14 | 000535-77-3 | 95 |
| 3 | Benzene, 2-ethyl-1,4-dimethyl- | 134 | C10H14 | 001758-88-9 | 95 |
| 4 | p-Cymene | 134 | C10H14 | 000099-87-6 | 95 |
| 5 | Benzene, 1-ethyl-3,5-dimethyl- | 134 | C10H14 | 000934-74-7 | 94 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

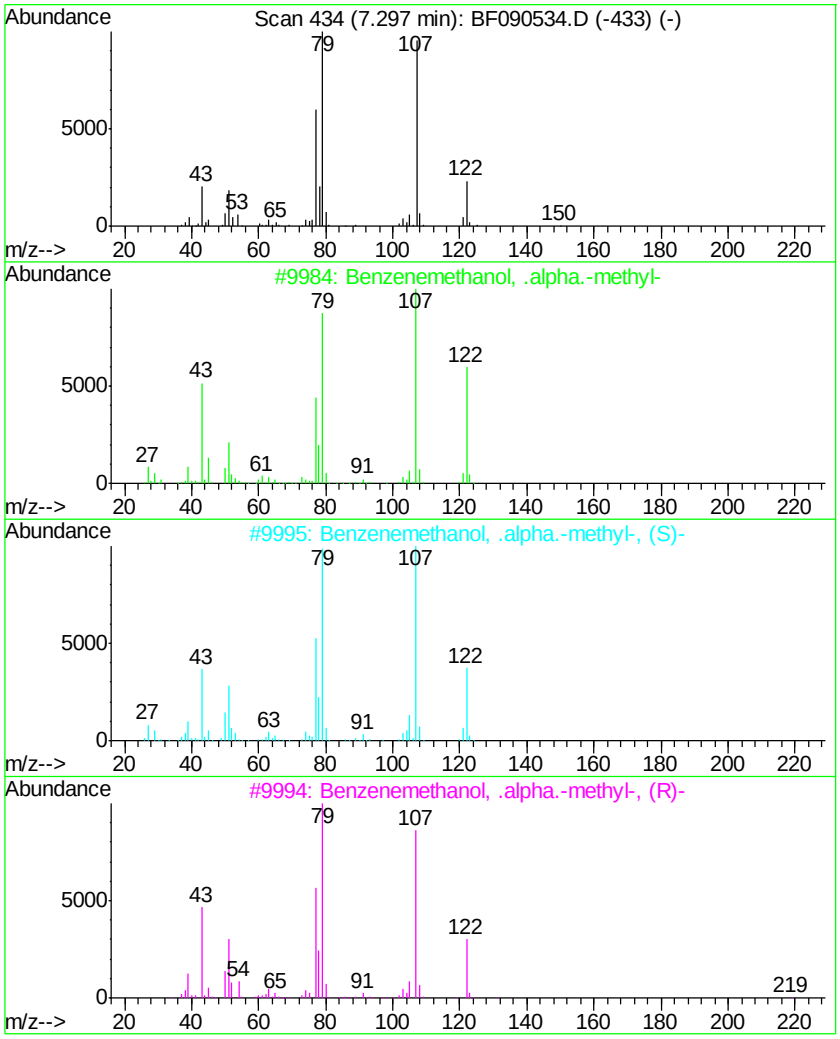
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

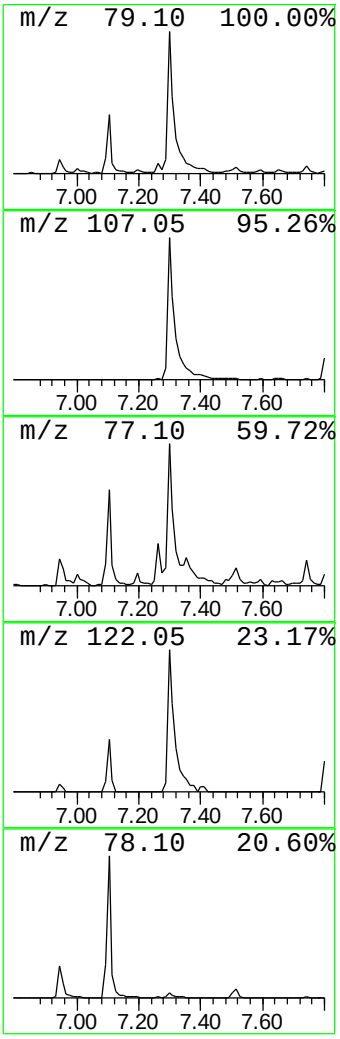
**********

Peak Number 5 Benzenemethanol, .alpha.-me... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.30 | 3.72 ng | 216757 | 1,4-Dichlorobenzene-d4 | 6.94 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenemethanol, .alpha.-methyl- | 122 | C8H10O | 000098-85-1 | 95 |
| 2 | Benzenemethanol, .alpha.-methyl-... | 122 | C8H10O | 001445-91-6 | 94 |
| 3 | Benzenemethanol, .alpha.-methyl-... | 122 | C8H10O | 001517-69-7 | 91 |
| 4 | Bicyclo[3.2.1]oct-2-ene, exo-4-(... | 248 | C14H16O2S | 1000142-99-0 | 64 |
| 5 | Propionic acid, 2,3-dihydroxy-3-... | 182 | C9H10O4 | 1000303-10-7 | 56 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

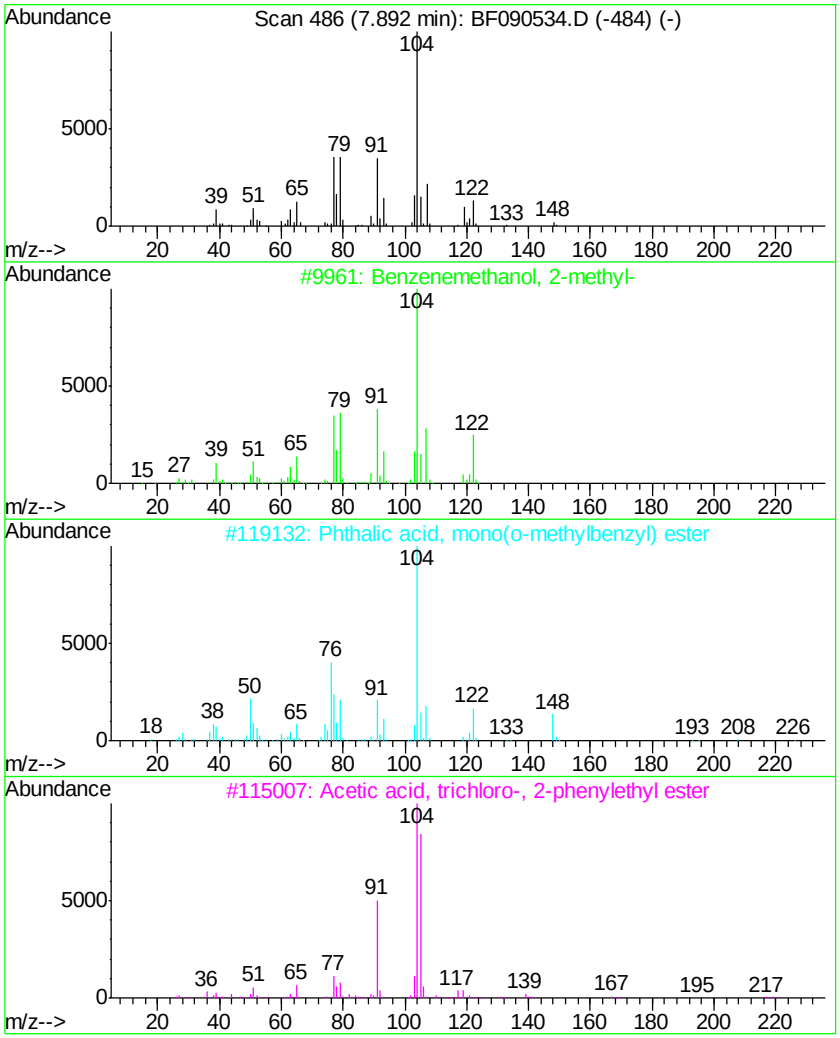
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

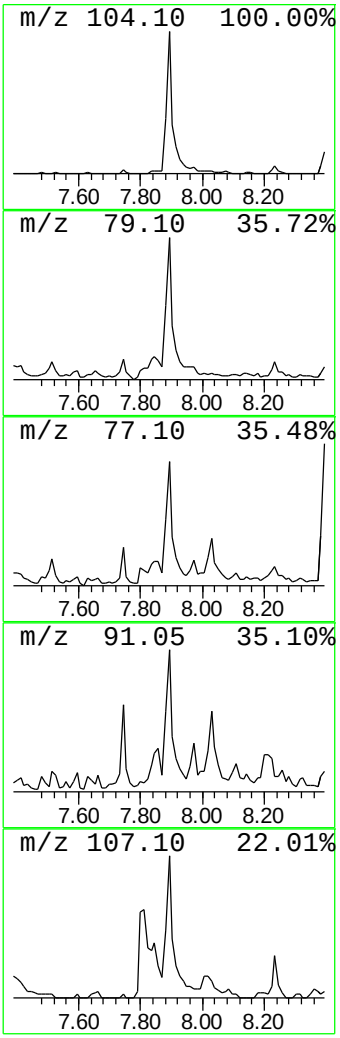
**********

Peak Number 6 Benzenemethanol, 2-methyl- Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.89 | 3.77 ng | 320922 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenemethanol, 2-methyl- | 122 | C8H10O | 000089-95-2 | 95 |
| 2 | Phthalic acid, mono(o-methylbenz... | 270 | C16H14O4 | 004619-49-2 | 59 |
| 3 | Acetic acid, trichloro-, 2-phenyl... | 266 | C10H9Cl3O2 | 071965-07-6 | 50 |
| 4 | Oxalic acid, 2-phenylethyl propy... | 236 | C13H16O4 | 1000309-65-5 | 50 |
| 5 | 1,3-Propanediamine, 2-phenyl- | 150 | C9H14N2 | 055165-09-8 | 47 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

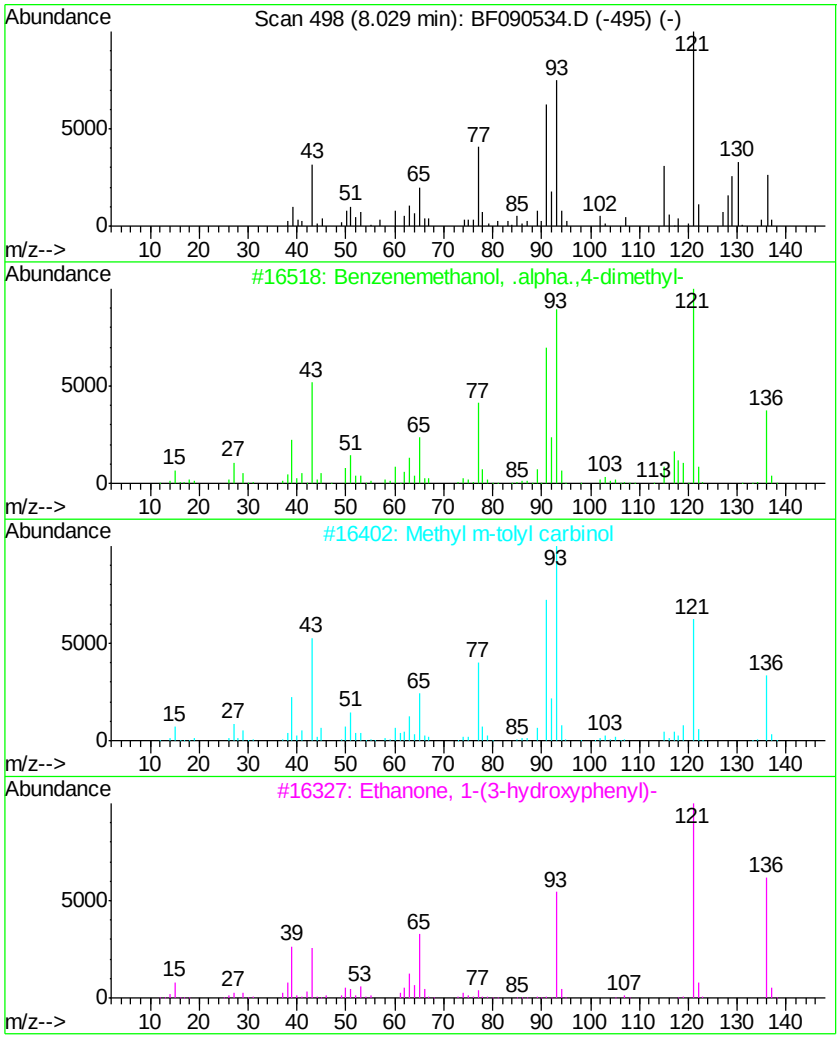
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

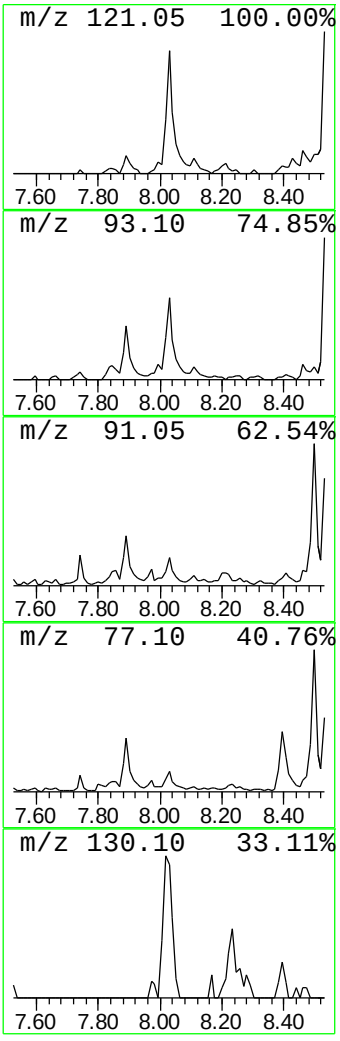
**********

Peak Number 7 Benzenemethanol, .alpha.,4-... Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.03 | 2.23 ng | 189659 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenemethanol, .alpha.,4-dimet... | 136 | C9H12O | 000536-50-5 | 89 |
| 2 | Methyl m-tolyl carbinol | 136 | C9H12O | 1000342-29-9 | 86 |
| 3 | Ethanone, 1-(3-hydroxyphenyl)- | 136 | C8H8O2 | 000121-71-1 | 60 |
| 4 | Bicyclo[2.2.1]hept-2-ene, 1,7,7-... | 136 | C10H16 | 000464-17-5 | 58 |
| 5 | Formamide, N-phenyl- | 121 | C7H7NO | 000103-70-8 | 53 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

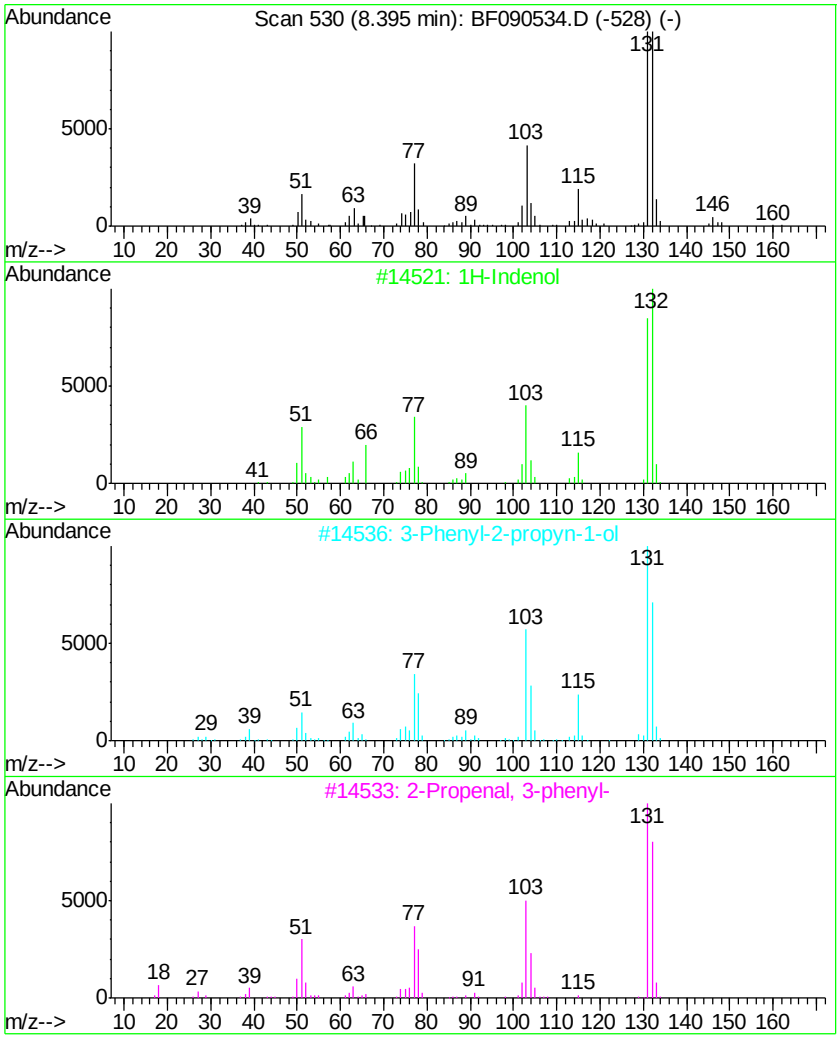
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

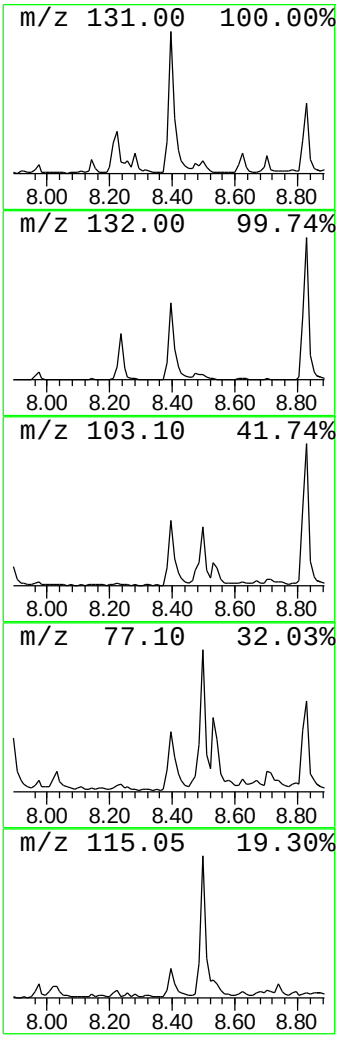
**********

Peak Number 8 1H-Indenol Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.39 | 5.87 ng | 500214 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Indenol | 132 | C9H8O | 056631-57-3 | 95 |
| 2 | 3-Phenyl-2-propyn-1-ol | 132 | C9H8O | 001504-58-1 | 90 |
| 3 | 2-Propenal, 3-phenyl- | 132 | C9H8O | 000104-55-2 | 87 |
| 4 | Benzofuran, 2-methyl- | 132 | C9H8O | 004265-25-2 | 81 |
| 5 | Benzene, (2-propynyloxy)- | 132 | C9H8O | 013610-02-1 | 72 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

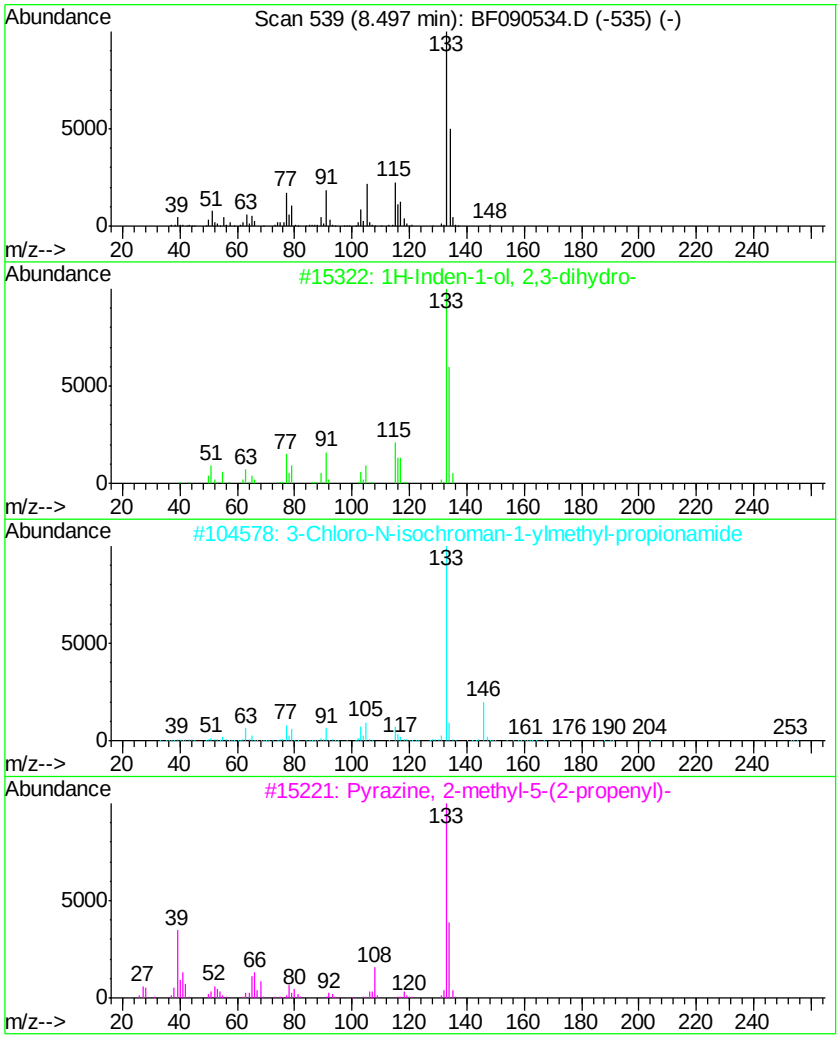
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

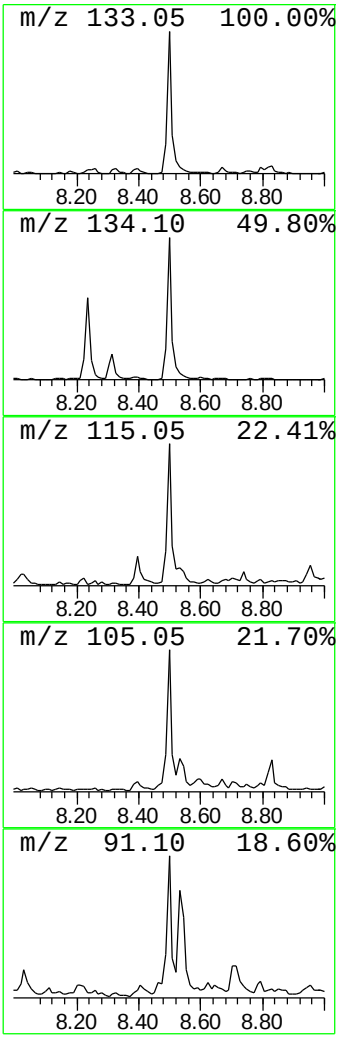
**********

Peak Number 9 1H-Inden-1-ol, 2,3-dihydro- Concentration Rank 4

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.50 | 13.75 ng | 1171400 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Inden-1-ol, 2,3-dihydro- | 134 | C9H10O | 006351-10-6 | 95 |
| 2 | 3-Chloro-N-isochroman-1-ylmethyl... | 253 | C13H16ClNO2 | 1000297-29-7 | 50 |
| 3 | Pyrazine, 2-methyl-5-(2-propenyl)- | 134 | C8H10N2 | 055138-63-1 | 49 |
| 4 | Pyrazine, 2-methyl-6-(1-propenyl... | 134 | C8H10N2 | 018217-81-7 | 49 |
| 5 | Pyrazine, 2-methyl-3-(2-propenyl)- | 134 | C8H10N2 | 055138-62-0 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

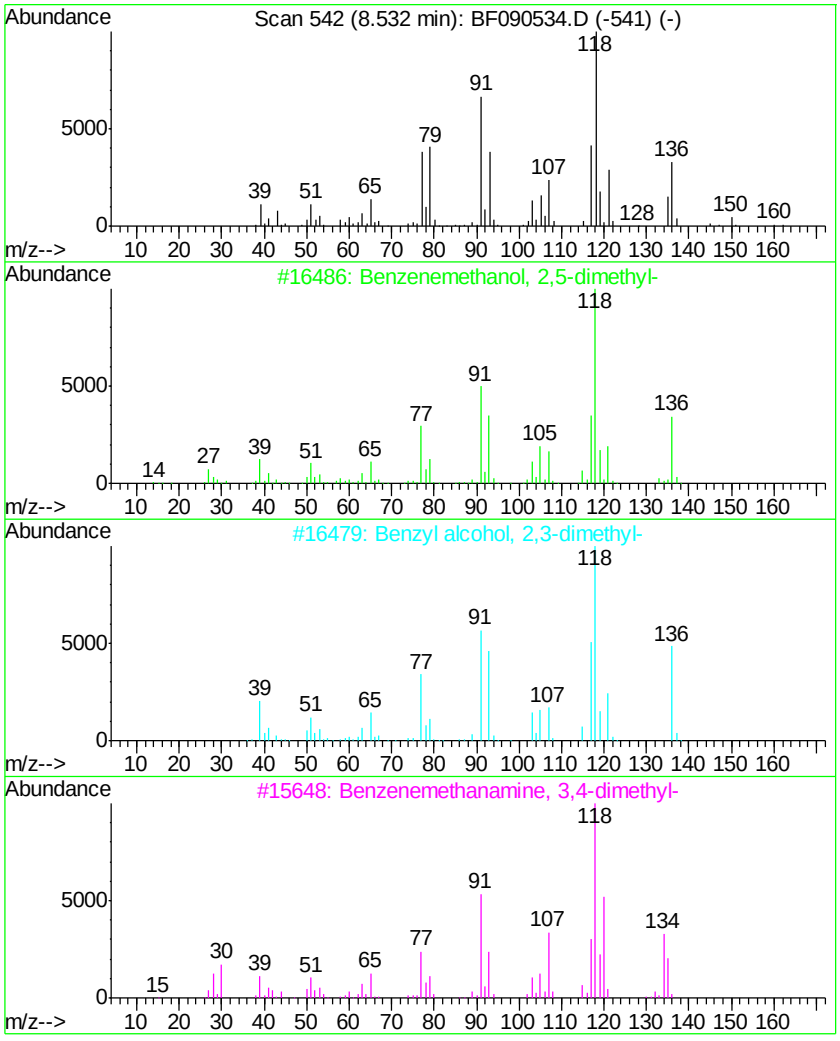
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

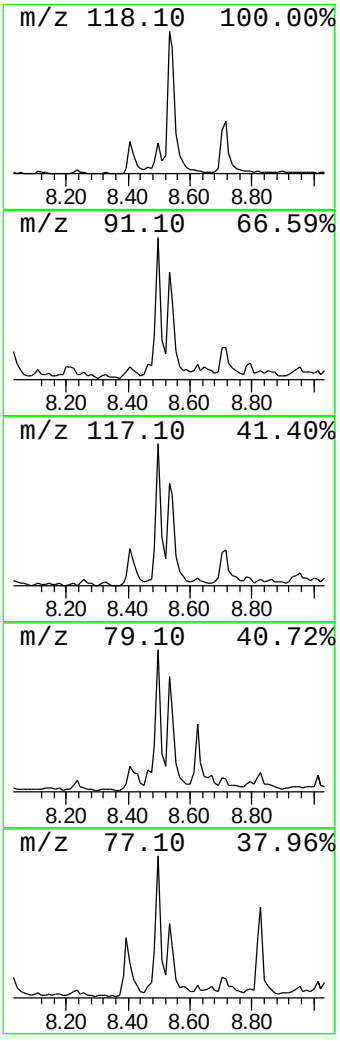
**********

Peak Number 10 Benzenemethanol, 2,5-dimethyl- Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.53 | 5.46 ng | 465324 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzenemethanol, 2,5-dimethyl- | 136 | C9H12O | 053957-33-8 | 93 |
| 2 | Benzyl alcohol, 2,3-dimethyl- | 136 | C9H12O | 013651-14-4 | 81 |
| 3 | Benzenemethanamine, 3,4-dimethyl- | 135 | C9H13N | 000102-48-7 | 53 |
| 4 | ,4-Dimethylbenzylamine | 135 | C9H13N | 000094-98-4 | 46 |
| 5 | 2,4-Nonadien-6-yn-1-ol, (E,E)- | 136 | C9H12O | 043212-86-8 | 43 |



# Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

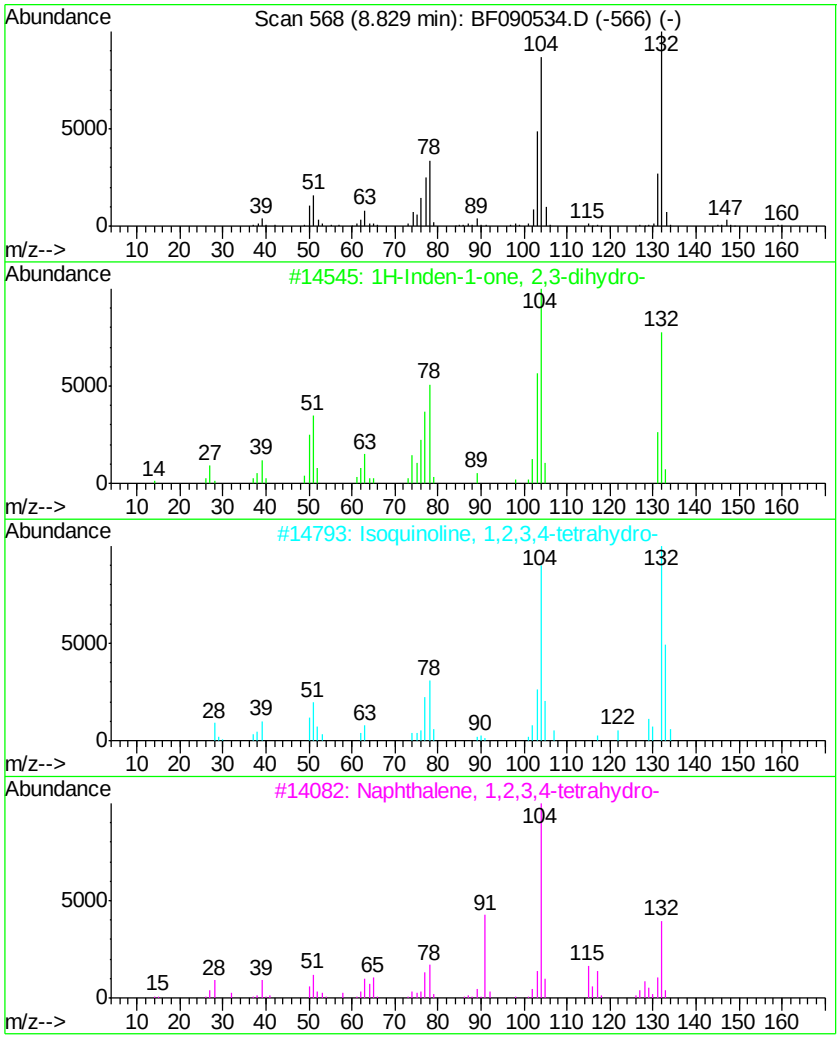
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

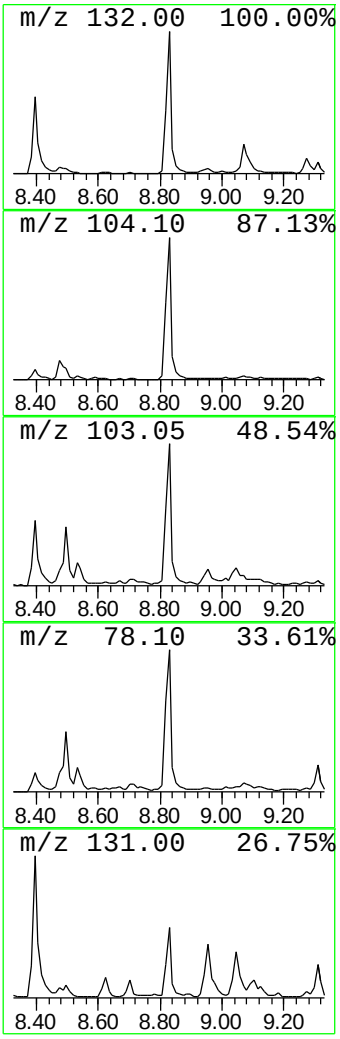
**********

Peak Number 11 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.83 | 6.81 ng | 579852 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1H-Inden-1-one, 2,3-dihydro- | 132 | C9H8O | 000083-33-0 | 94 |
| 2 | Isoquinoline, 1,2,3,4-tetrahydro- | 133 | C9H11N | 000091-21-4 | 64 |
| 3 | Naphthalene, 1,2,3,4-tetrahydro- | 132 | C10H12 | 000119-64-2 | 64 |
| 4 | 2H-Inden-2-one, 1,3-dihydro- | 132 | C9H8O | 000615-13-4 | 59 |
| 5 | Styrene | 104 | C8H8 | 000100-42-5 | 55 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

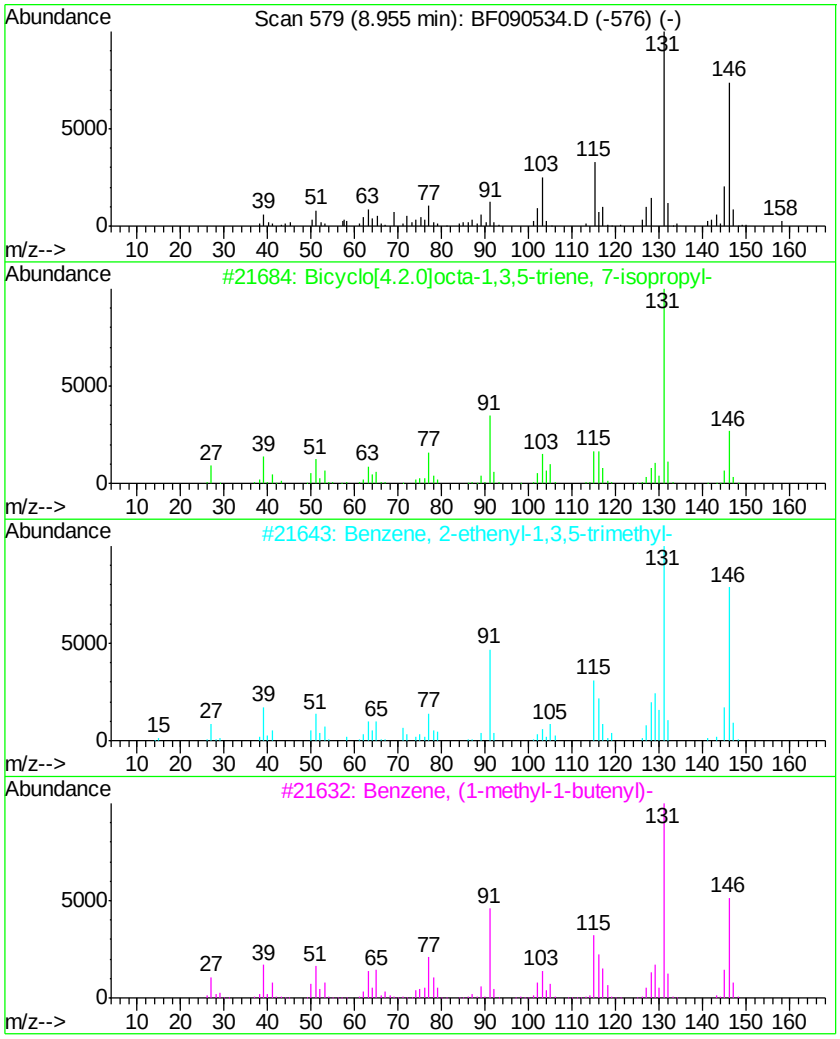
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

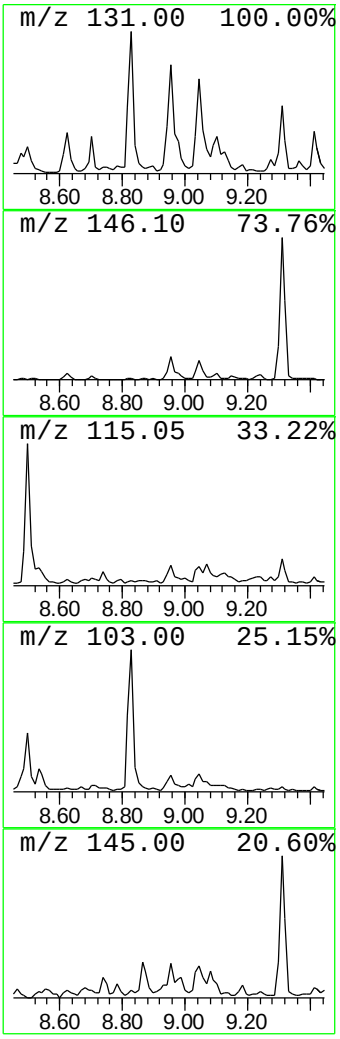
**********

Peak Number 12 Bicyclo[4.2.0]octa-1,3,5-tr... Concentration Rank 19

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 8.95 | 2.22 ng | 189394 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 146 | C11H14 | 027087-54-3 | 86 |
| 2 | Benzene, 2-ethenyl-1,3,5-trimethyl- | 146 | C11H14 | 000769-25-5 | 83 |
| 3 | Benzene, (1-methyl-1-butenyl)- | 146 | C11H14 | 053172-84-2 | 83 |
| 4 | 1H-Inden-1-one, 2,3-dihydro-3-me... | 146 | C10H10O | 006072-57-7 | 83 |
| 5 | Benzene, (1,2-dimethyl-1-propenyl)- | 146 | C11H14 | 000769-57-3 | 80 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

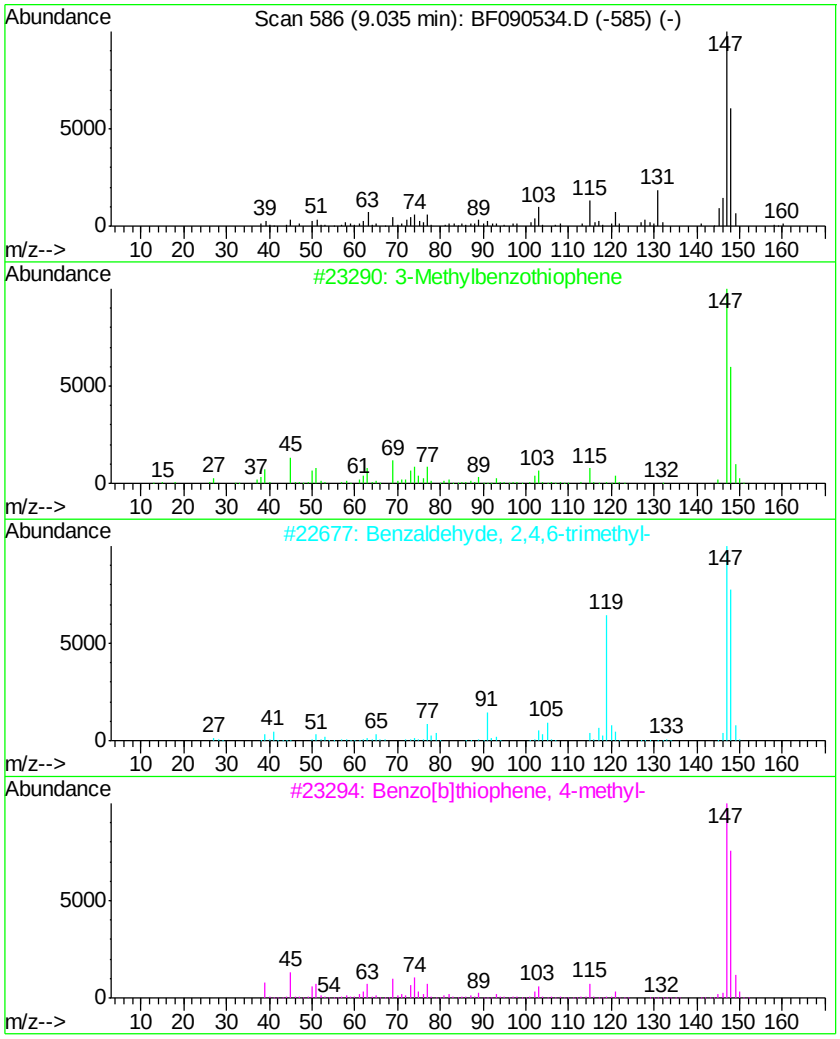
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

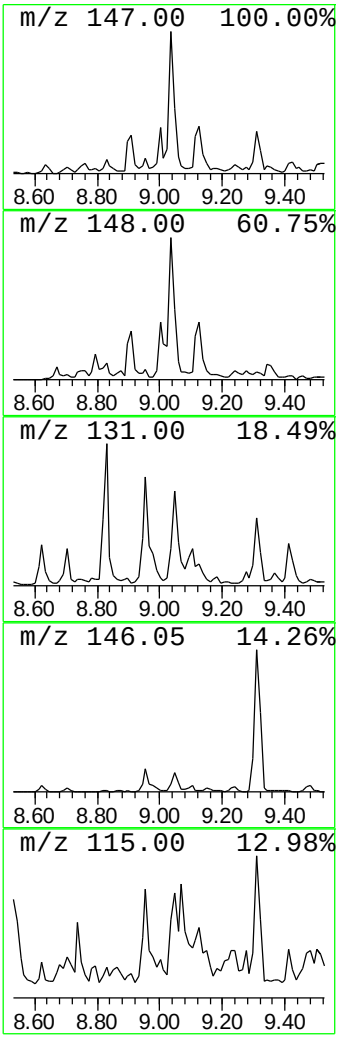
**********

Peak Number 13 3-Methylbenzothiophene Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.03 | 3.08 ng | 262768 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Methylbenzothiophene | 148 | C9H8S | 001455-18-1 | 64 |
| 2 | Benzaldehyde, 2,4,6-trimethyl- | 148 | C10H12O | 000487-68-3 | 59 |
| 3 | Benzo[b]thiophene, 4-methyl- | 148 | C9H8S | 014315-11-8 | 50 |
| 4 | Benzo[b]thiophene, 5-methyl- | 148 | C9H8S | 014315-14-1 | 50 |
| 5 | Pyridine, 4-(1-pyrrolidinyl)- | 148 | C9H12N2 | 002456-81-7 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

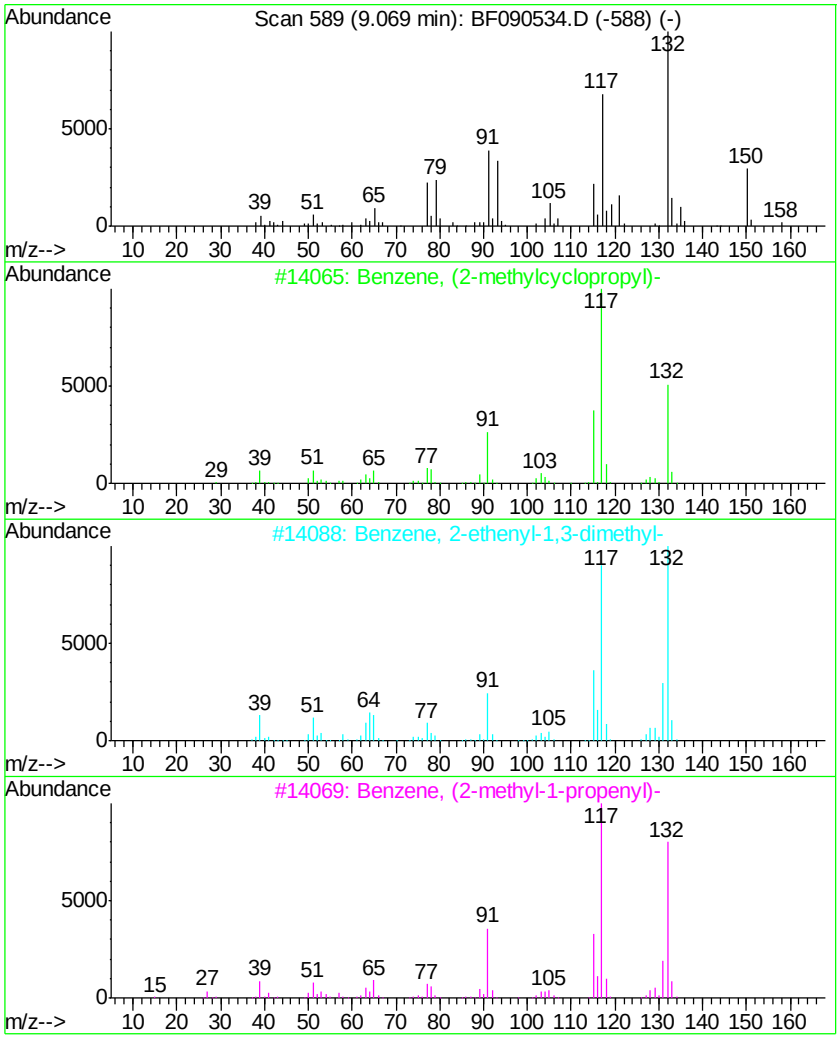
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

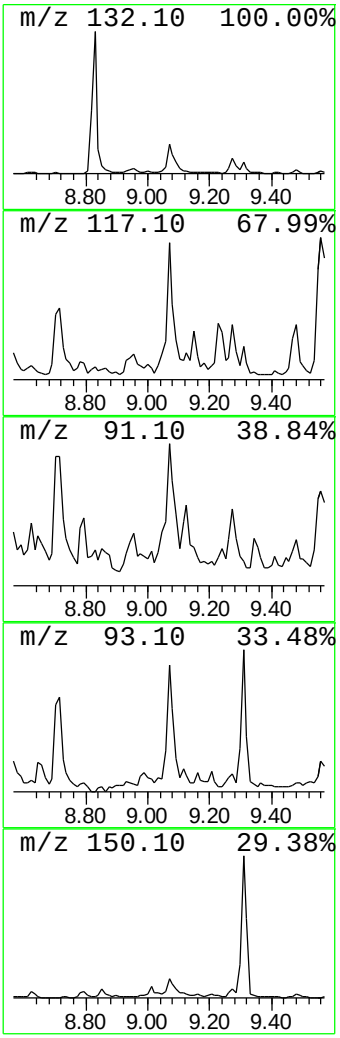
**********

Peak Number 14 Benzene, (2-methylcycloprop... Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.07 | 3.07 ng | 261853 | Naphthalene-d8 | 8.23 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, (2-methylcyclopropyl)- | 132 | C10H12 | 1000327-39-0 | 53 |
| 2 | Benzene, 2-ethenyl-1,3-dimethyl- | 132 | C10H12 | 002039-90-9 | 49 |
| 3 | Benzene, (2-methyl-1-propenyl)- | 132 | C10H12 | 000768-49-0 | 49 |
| 4 | Benzene, 1-methyl-4-(2-propenyl)- | 132 | C10H12 | 003333-13-9 | 49 |
| 5 | Benzene, 1-ethenyl-3-ethyl- | 132 | C10H12 | 007525-62-4 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

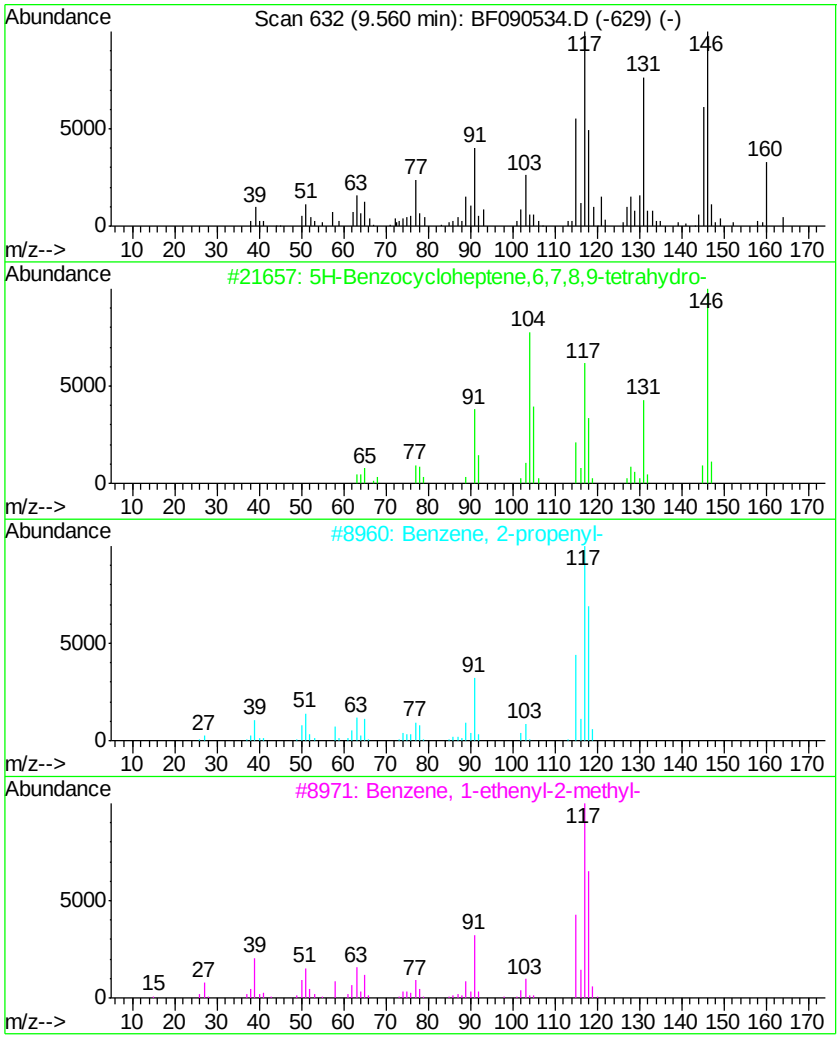
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

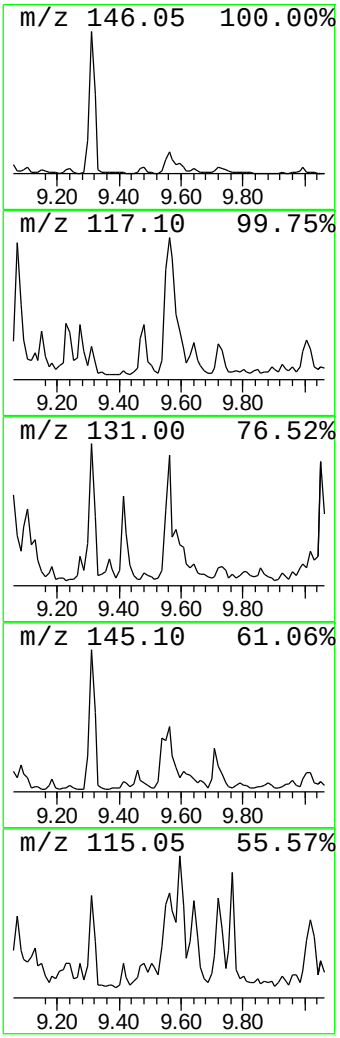
**********

Peak Number 15 5H-Benzocycloheptene,6,7,8,... Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.56 | 5.04 ng | 524481 | Acenaphthene-d10 | 9.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5H-Benzocycloheptene,6,7,8,9-tet... | 146 | C11H14 | 001075-16-7 | 76 |
| 2 | Benzene, 2-propenyl- | 118 | C9H10 | 000300-57-2 | 64 |
| 3 | Benzene, 1-ethenyl-2-methyl- | 118 | C9H10 | 000611-15-4 | 64 |
| 4 | 2,3,4,5,6,7-Hexahydro-1H-cyclope... | 146 | C11H14 | 1000189-31-0 | 62 |
| 5 | 7-Methylindan-1-one | 146 | C10H10O | 039627-61-7 | 60 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

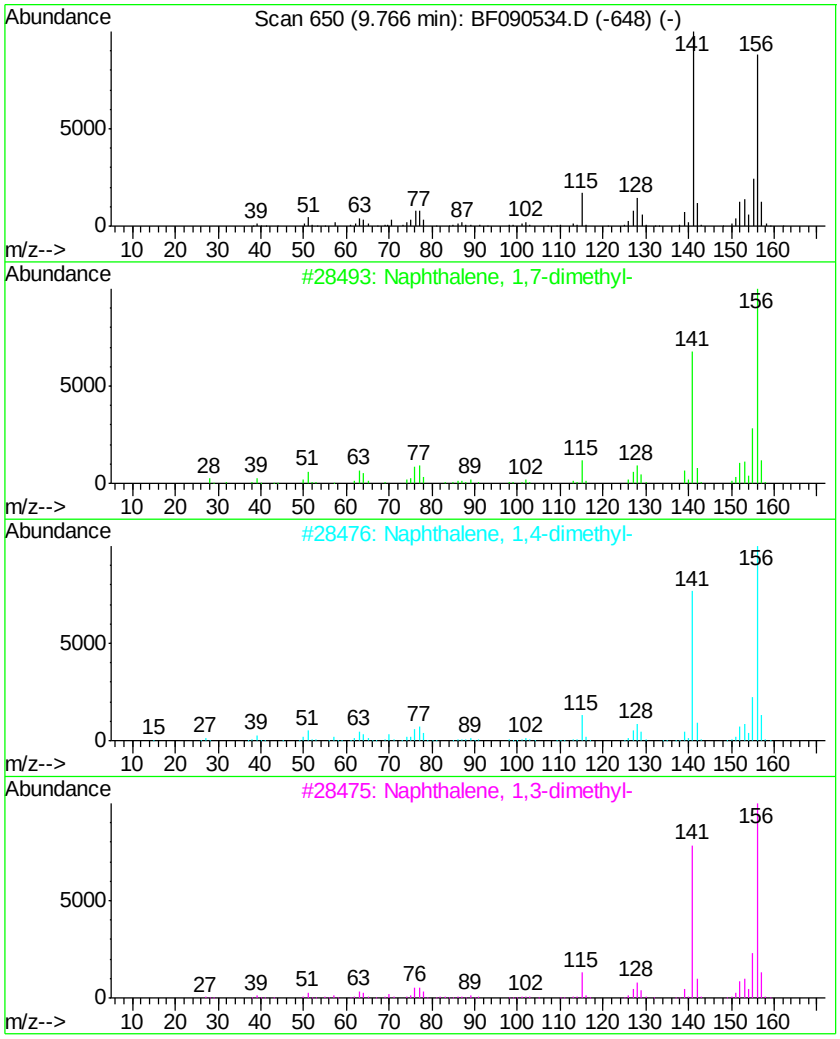
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

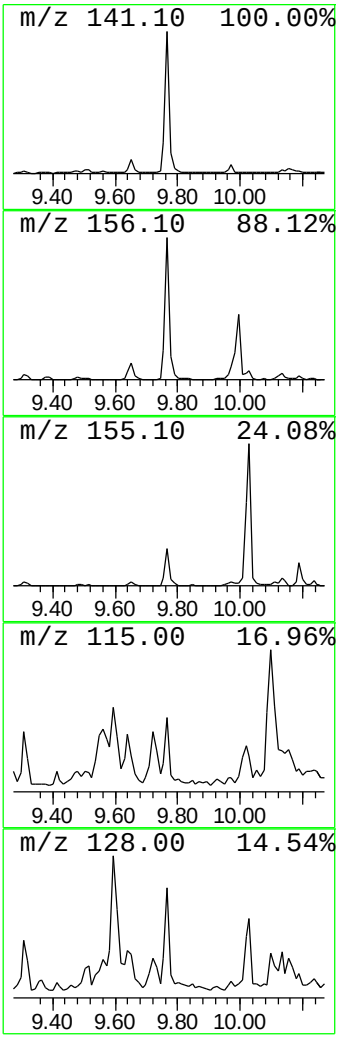
**********

Peak Number 16 Naphthalene, 1,7-dimethyl- Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.77 | 2.22 ng | 230583 | Acenaphthene-d10 | 9.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Naphthalene, 1,7-dimethyl- | 156 | C12H12 | 000575-37-1 | 97 |
| 2 | Naphthalene, 1,4-dimethyl- | 156 | C12H12 | 000571-58-4 | 97 |
| 3 | Naphthalene, 1,3-dimethyl- | 156 | C12H12 | 000575-41-7 | 96 |
| 4 | Naphthalene, 1,5-dimethyl- | 156 | C12H12 | 000571-61-9 | 96 |
| 5 | Naphthalene, 1,6-dimethyl- | 156 | C12H12 | 000575-43-9 | 96 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

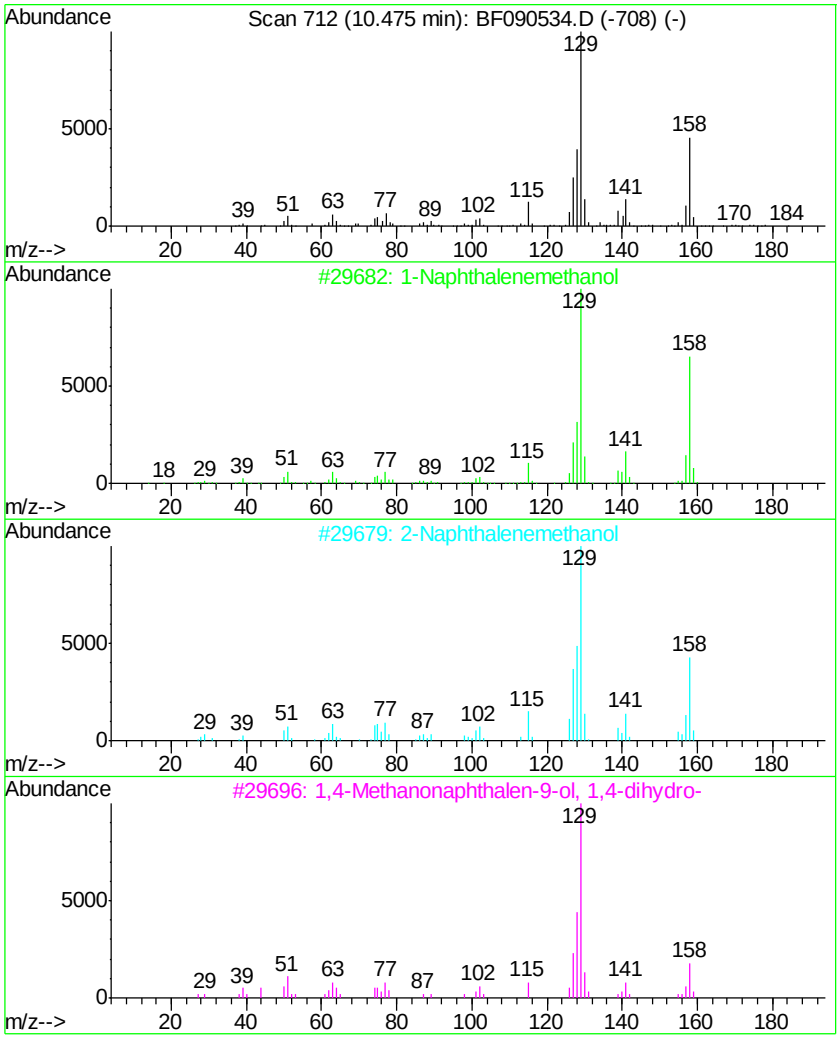
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

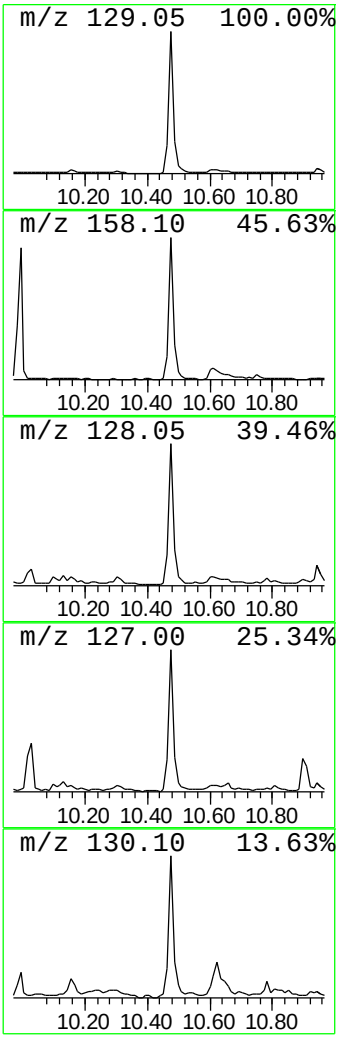
**********

Peak Number 17 1-Naphthalenemethanol Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.47 | 9.04 ng | 940033 | Acenaphthene-d10 | 9.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Naphthalenemethanol | 158 | C11H10O | 004780-79-4 | 94 |
| 2 | 2-Naphthalenemethanol | 158 | C11H10O | 001592-38-7 | 94 |
| 3 | 1,4-Methanonaphthalen-9-ol, 1,4-... | 158 | C11H10O | 004796-33-2 | 83 |
| 4 | Benzene, 1,3-hexadienyl- | 158 | C12H14 | 041635-77-2 | 72 |
| 5 | 1-butyne, 4-chloro-3-methyl-3-ph... | 178 | C11H11Cl | 1000161-45-9 | 50 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

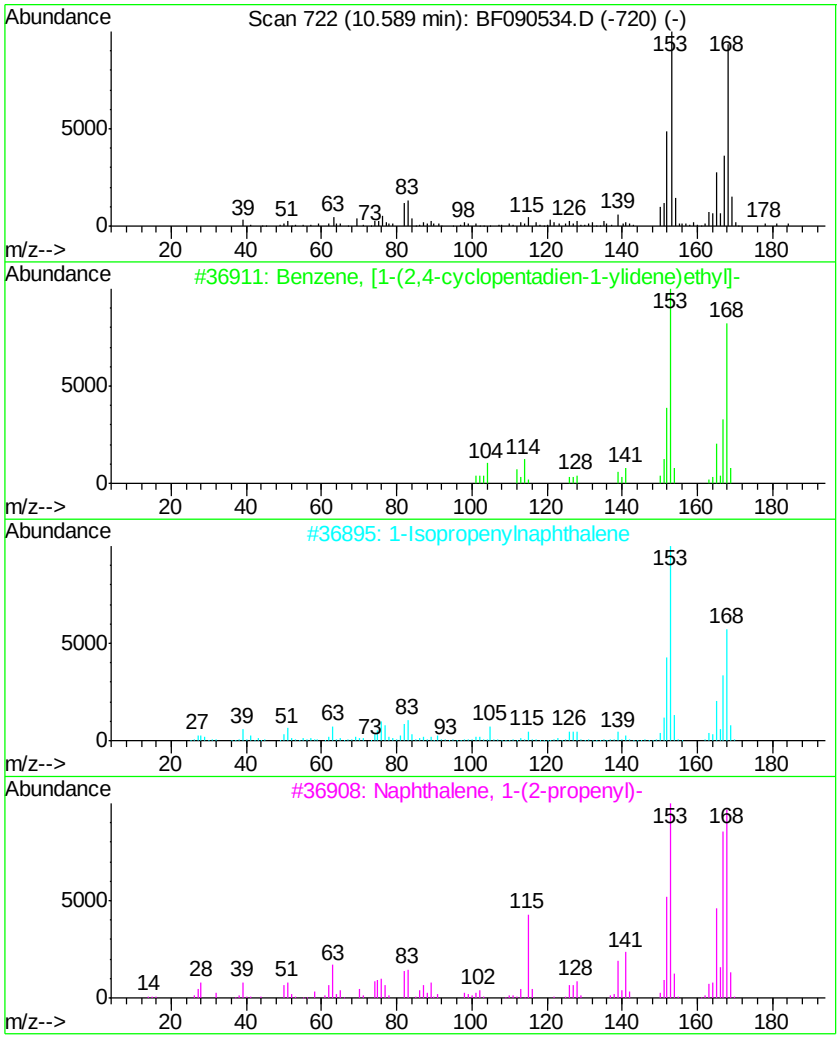
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

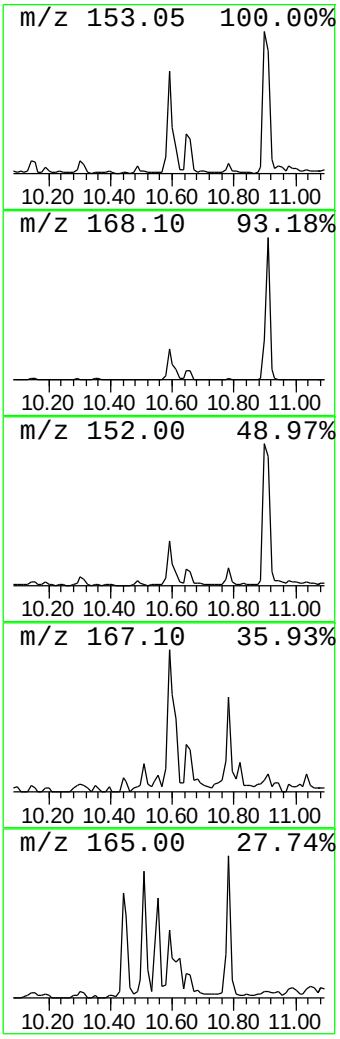
**********

Peak Number 18 Benzene, [1-(2,4-cyclopenta... Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.59 | 3.68 ng | 382612 | Acenaphthene-d10 | 9.99 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzene, [1-(2,4-cyclopentadien-... | 168 | C13H12 | 002320-32-3 | 90 |
| 2 | 1-Isopropenylnaphthalene | 168 | C13H12 | 001855-47-6 | 74 |
| 3 | Naphthalene, 1-(2-propenyl)- | 168 | C13H12 | 002489-86-3 | 64 |
| 4 | Naphthalene, 2-(1-methylethenyl)- | 168 | C13H12 | 003710-23-4 | 59 |
| 5 | Ethanone, 1-(2,3,4-trihydroxyphe... | 168 | C8H8O4 | 000528-21-2 | 52 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

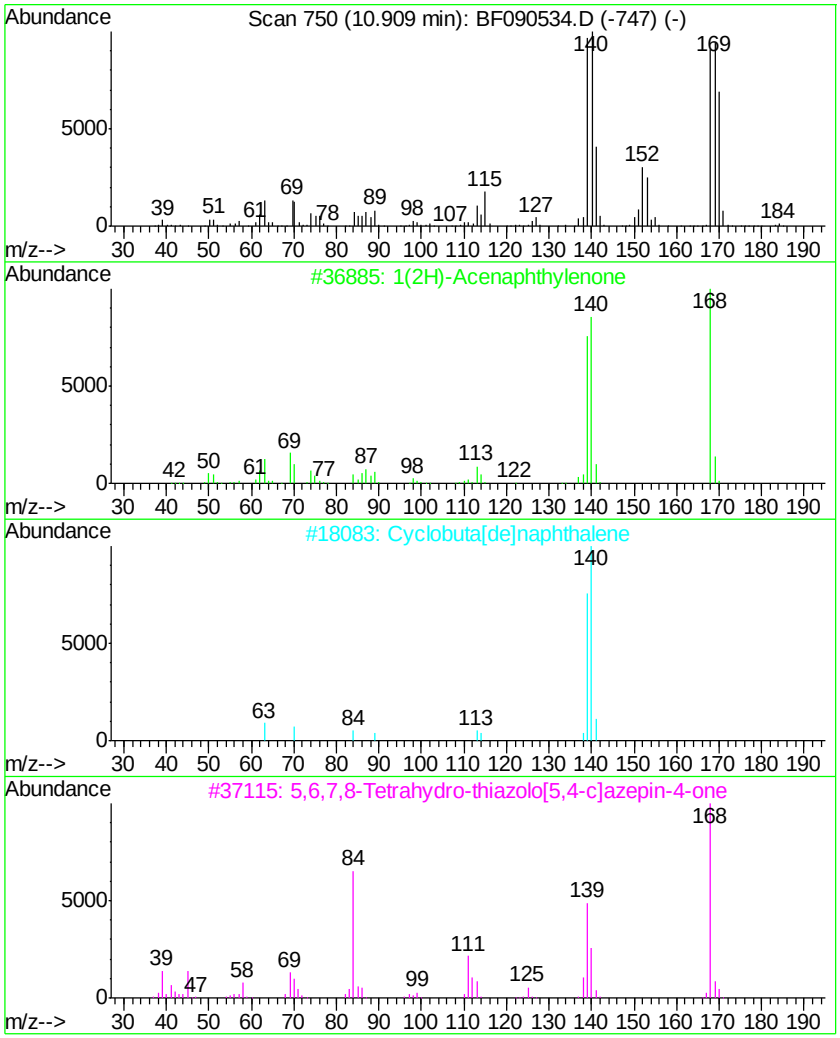
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

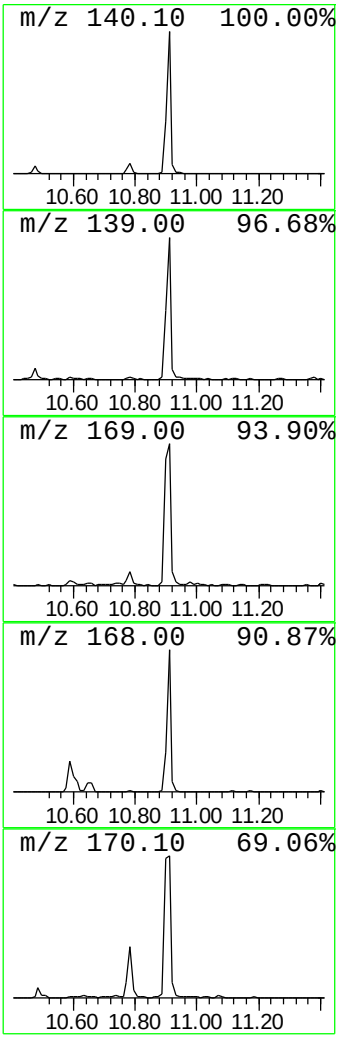
**********

Peak Number 19 1(2H)-Acenaphthylenone Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.91 | 17.44 ng | 1668670 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1(2H)-Acenaphthylenone | 168 | C12H8O | 002235-15-6 | 91 |
| 2 | Cyclobuta[de]naphthalene | 140 | C11H8 | 024973-91-9 | 38 |
| 3 | 5,6,7,8-Tetrahydro-thiazolo[5,4-... | 168 | C7H8N2OS | 1000317-75-4 | 35 |
| 4 | Dibenzofuran | 168 | C12H8O | 000132-64-9 | 30 |
| 5 | 1H-Inden-1-ol, 4,7-difluoro-2,3-... | 170 | C9H8F2O | 130408-17-2 | 30 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

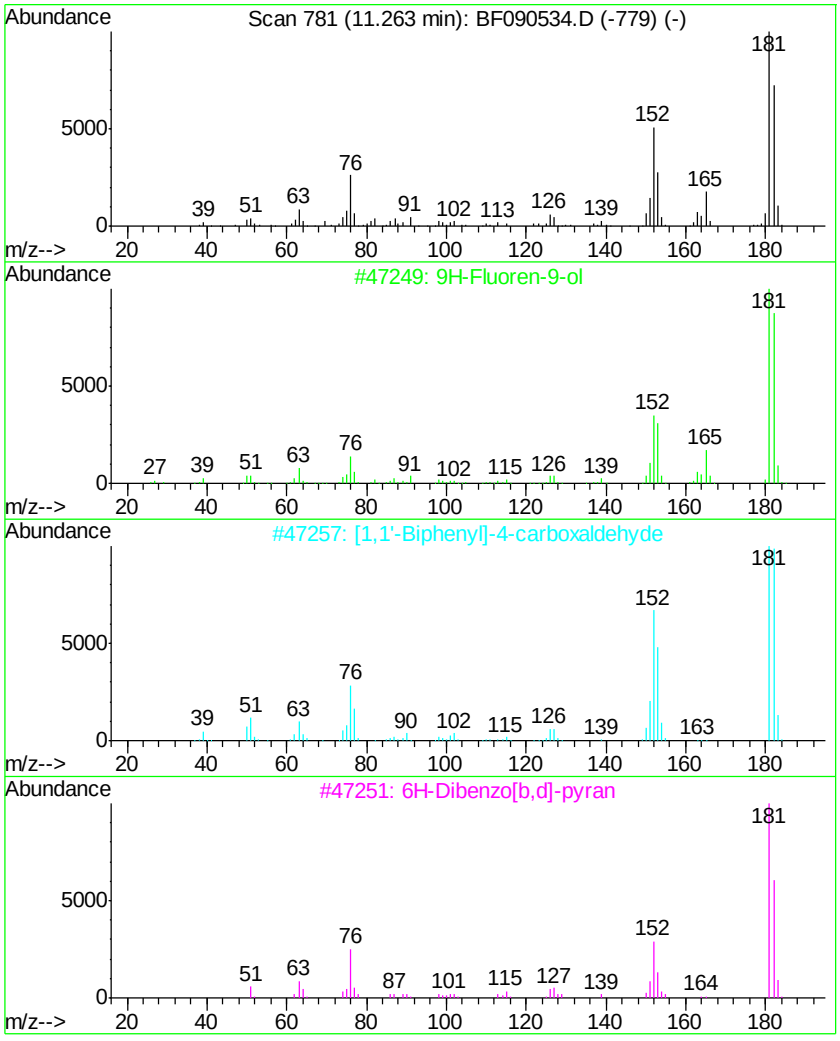
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

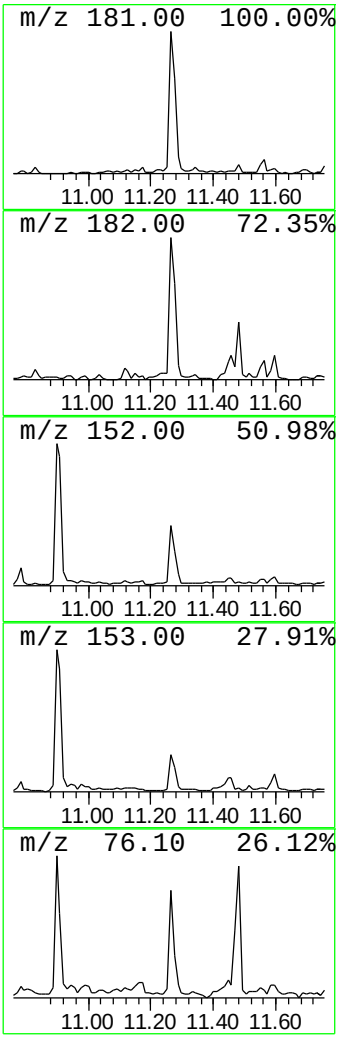
**********

Peak Number 20 9H-Fluoren-9-ol Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.26 | 2.53 ng | 242220 | Phenanthrene-d10 | 11.48 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9H-Fluoren-9-ol | 182 | C13H10O | 001689-64-1 | 96 |
| 2 | [1,1'-Biphenyl]-4-carboxaldehyde | 182 | C13H10O | 003218-36-8 | 86 |
| 3 | 6H-Dibenzo[b,d]-pyran | 182 | C13H10O | 000229-95-8 | 83 |
| 4 | 3-(1-Naphthyl)acrylaldehyde | 182 | C13H10O | 001504-73-0 | 81 |
| 5 | 3-(2-Naphthyl)acrylaldehyde | 182 | C13H10O | 020884-05-3 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101216\
Data File : BF090534.D
Acq On : 12 Oct 2016 14:43
Operator : UM/SJ
Sample : H5153-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** AOU2-MW1-100716

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

| | | | | | Internal Standard | | | |
|---|---|---|---|---|---|---|---|---|
| TIC Top Hit name | RT | EstConc | Units | Response | # | RT | Resp | Conc |
| 2-Pentanone, 4-hy... | 5.14 | 6.4 | ng | 371671 | 1 | 6.94 | 1166810 | 20.0 |
| unknown6.71 | 6.71 | 57.1 | ng | 3332820 | 1 | 6.94 | 1166810 | 20.0 |
| o-Cymene | 7.26 | 4.7 | ng | 272206 | 1 | 6.94 | 1166810 | 20.0 |
| Benzenemethanol, ... | 7.30 | 3.7 | ng | 216757 | 1 | 6.94 | 1166810 | 20.0 |
| Benzenemethanol, ... | 7.89 | 3.8 | ng | 320922 | 2 | 8.23 | 1704100 | 20.0 |
| Benzenemethanol, ... | 8.03 | 2.2 | ng | 189659 | 2 | 8.23 | 1704100 | 20.0 |
| 1H-Indenol | 8.39 | 5.9 | ng | 500214 | 2 | 8.23 | 1704100 | 20.0 |
| 1H-Inden-1-ol, 2,... | 8.50 | 13.8 | ng | 1171400 | 2 | 8.23 | 1704100 | 20.0 |
| Benzenemethanol, ... | 8.53 | 5.5 | ng | 465324 | 2 | 8.23 | 1704100 | 20.0 |
| 1H-Inden-1-one, 2... | 8.83 | 6.8 | ng | 579852 | 2 | 8.23 | 1704100 | 20.0 |
| Bicyclo[4.2.0]oct... | 8.95 | 2.2 | ng | 189394 | 2 | 8.23 | 1704100 | 20.0 |
| 3-Methylbenzothio... | 9.03 | 3.1 | ng | 262768 | 2 | 8.23 | 1704100 | 20.0 |
| Benzene, (2-methy... | 9.07 | 3.1 | ng | 261853 | 2 | 8.23 | 1704100 | 20.0 |
| 5H-Benzocyclohept... | 9.56 | 5.0 | ng | 524481 | 3 | 9.99 | 2079240 | 20.0 |
| Naphthalene, 1,7-... | 9.77 | 2.2 | ng | 230583 | 3 | 9.99 | 2079240 | 20.0 |
| 1-Naphthalenemeth... | 10.47 | 9.0 | ng | 940033 | 3 | 9.99 | 2079240 | 20.0 |
| Benzene, [1-(2,4-... | 10.59 | 3.7 | ng | 382612 | 3 | 9.99 | 2079240 | 20.0 |
| 1(2H)-Acenaphthyl... | 10.91 | 17.4 | ng | 1668670 | 4 | 11.48 | 1913180 | 20.0 |
| 9H-Fluoren-9-ol | 11.26 | 2.5 | ng | 242220 | 4 | 11.48 | 1913180 | 20.0 |