LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

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-BF121716.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 | 3.527 | 123 | 126 | 131 | rVB | 87996 | 165993 | 1.74% | 0.218% |
| 2 | 3.710 | 140 | 142 | 151 | rVB | 63867 | 119756 | 1.25% | 0.158% |
| 3 | 4.933 | 246 | 249 | 258 | rVB | 1006189 | 1260574 | 13.20% | 1.659% |
| 4 | 5.367 | 284 | 287 | 289 | rBV | 4630495 | 4470306 | 46.82% | 5.883% |
| 5 | 6.407 | 375 | 378 | 380 | rBV | 2782866 | 2626405 | 27.51% | 3.456% |
| 6 | 6.533 | 386 | 389 | 391 | rBV | 5078149 | 6417544 | 67.21% | 8.445% |
| 7 | 6.761 | 407 | 409 | 412 | rBV | 1518640 | 1696125 | 17.76% | 2.232% |
| 8 | 6.922 | 420 | 423 | 426 | rBV | 5204062 | 5796204 | 60.70% | 7.628% |
| 9 | 7.116 | 437 | 440 | 442 | rBV | 101035 | 136505 | 1.43% | 0.180% |
| 10 | 7.287 | 451 | 455 | 456 | rBV | 70013 | 118382 | 1.24% | 0.156% |
| 11 | 7.333 | 456 | 459 | 461 | rVV | 4100130 | 5001432 | 52.38% | 6.582% |
| 12 | 7.367 | 461 | 462 | 464 | rVV | 309923 | 287100 | 3.01% | 0.378% |
| 13 | 7.413 | 464 | 466 | 468 | rVV3 | 184491 | 241860 | 2.53% | 0.318% |
| 14 | 7.459 | 468 | 470 | 472 | rVV2 | 119878 | 163469 | 1.71% | 0.215% |
| 15 | 7.516 | 472 | 475 | 477 | rVV | 77538 | 166082 | 1.74% | 0.219% |
| 16 | 7.584 | 479 | 481 | 483 | rBV2 | 82958 | 138229 | 1.45% | 0.182% |
| 17 | 7.710 | 489 | 492 | 496 | rVB4 | 50602 | 101449 | 1.06% | 0.134% |
| 18 | 7.790 | 496 | 499 | 503 | rBV5 | 82581 | 194862 | 2.04% | 0.256% |
| 19 | 7.996 | 515 | 517 | 519 | rVV2 | 96463 | 115589 | 1.21% | 0.152% |
| 20 | 8.053 | 519 | 522 | 524 | rVV | 2610885 | 2518292 | 26.37% | 3.314% |
| 21 | 8.099 | 524 | 526 | 532 | rVB4 | 85925 | 141823 | 1.49% | 0.187% |
| 22 | 8.213 | 532 | 536 | 537 | rBV2 | 82259 | 108497 | 1.14% | 0.143% |
| 23 | 8.430 | 551 | 555 | 557 | rVB5 | 80693 | 197205 | 2.07% | 0.260% |
| 24 | 8.533 | 562 | 564 | 567 | rVB3 | 93350 | 133963 | 1.40% | 0.176% |
| 25 | 8.590 | 567 | 569 | 570 | rBV | 95419 | 128970 | 1.35% | 0.170% |
| 26 | 8.613 | 570 | 571 | 574 | rVB3 | 70076 | 116471 | 1.22% | 0.153% |
| 27 | 8.762 | 581 | 584 | 585 | rBV3 | 47246 | 108739 | 1.14% | 0.143% |
| 28 | 8.796 | 585 | 587 | 589 | rVB3 | 85452 | 96033 | 1.01% | 0.126% |
| 29 | 8.899 | 594 | 596 | 599 | rVB4 | 71416 | 134321 | 1.41% | 0.177% |
| 30 | 9.047 | 607 | 609 | 611 | rVB2 | 79231 | 104080 | 1.09% | 0.137% |
| 31 | 9.139 | 613 | 617 | 619 | rVV | 7278131 | 9548181 | 100.00% | 12.565% |
| 32 | 9.230 | 622 | 625 | 628 | rBV5 | 70498 | 175293 | 1.84% | 0.231% |
| 33 | 9.436 | 641 | 643 | 644 | rBV2 | 76249 | 118702 | 1.24% | 0.156% |
| 34 | 9.470 | 644 | 646 | 647 | rVV | 205401 | 264309 | 2.77% | 0.348% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

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-BF121716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 35 | 9.505 | 647 | 649 | 650 | rVV | 168444 | 235867 | 2.47% | 0.310% |
| 36 | 9.573 | 653 | 655 | 657 | rVV2 | 154968 | 308402 | 3.23% | 0.406% |
| 37 | 9.619 | 657 | 659 | 661 | rVV2 | 287037 | 429221 | 4.50% | 0.565% |
| 38 | 9.665 | 661 | 663 | 665 | rVB3 | 106741 | 148470 | 1.55% | 0.195% |
| 39 | 9.802 | 671 | 675 | 678 | rBV | 2500111 | 2586435 | 27.09% | 3.404% |
| 40 | 10.008 | 687 | 693 | 694 | rBV6 | 137421 | 355732 | 3.73% | 0.468% |
| 41 | 10.042 | 694 | 696 | 697 | rVB2 | 143052 | 159374 | 1.67% | 0.210% |
| 42 | 10.099 | 699 | 701 | 704 | rVV2 | 163945 | 387428 | 4.06% | 0.510% |
| 43 | 10.156 | 704 | 706 | 710 | rVB4 | 164952 | 270971 | 2.84% | 0.357% |
| 44 | 10.499 | 732 | 736 | 737 | rBV4 | 145965 | 253263 | 2.65% | 0.333% |
| 45 | 10.545 | 737 | 740 | 742 | rVV | 598897 | 874536 | 9.16% | 1.151% |
| 46 | 10.602 | 742 | 745 | 747 | rVV | 3621575 | 5554793 | 58.18% | 7.310% |
| 47 | 10.636 | 747 | 748 | 751 | rVB3 | 103889 | 100897 | 1.06% | 0.133% |
| 48 | 10.705 | 751 | 754 | 757 | rBV2 | 256691 | 399040 | 4.18% | 0.525% |
| 49 | 11.116 | 788 | 790 | 791 | rBV | 69264 | 109614 | 1.15% | 0.144% |
| 50 | 11.139 | 791 | 792 | 795 | rVB3 | 311372 | 409082 | 4.28% | 0.538% |
| 51 | 11.288 | 802 | 805 | 807 | rBV | 2573885 | 2443352 | 25.59% | 3.215% |
| 52 | 11.368 | 810 | 812 | 814 | rVV | 443914 | 473133 | 4.96% | 0.623% |
| 53 | 11.402 | 814 | 815 | 821 | rVB4 | 87352 | 118400 | 1.24% | 0.156% |
| 54 | 11.562 | 827 | 829 | 830 | rVV | 109963 | 143492 | 1.50% | 0.189% |
| 55 | 11.585 | 830 | 831 | 835 | rVB | 148956 | 198904 | 2.08% | 0.262% |
| 56 | 11.745 | 843 | 845 | 846 | rBV2 | 83844 | 99253 | 1.04% | 0.131% |
| 57 | 11.768 | 846 | 847 | 850 | rVB | 113462 | 146700 | 1.54% | 0.193% |
| 58 | 11.825 | 850 | 852 | 861 | rVB3 | 219211 | 387291 | 4.06% | 0.510% |
| 59 | 11.951 | 861 | 863 | 865 | rBV | 327777 | 368353 | 3.86% | 0.485% |
| 60 | 12.613 | 919 | 921 | 923 | rBV2 | 157672 | 198998 | 2.08% | 0.262% |
| 61 | 12.705 | 927 | 929 | 931 | rVB | 1728865 | 1480667 | 15.51% | 1.949% |
| 62 | 12.785 | 931 | 936 | 938 | rVB2 | 218371 | 371606 | 3.89% | 0.489% |
| 63 | 12.876 | 941 | 944 | 947 | rBV | 6404026 | 7297446 | 76.43% | 9.603% |
| 64 | 13.414 | 988 | 991 | 992 | rBV | 842710 | 1068197 | 11.19% | 1.406% |
| 65 | 13.448 | 992 | 994 | 996 | rBV2 | 130940 | 242119 | 2.54% | 0.319% |
| 66 | 13.779 | 1021 | 1023 | 1031 | rVB | 225400 | 280035 | 2.93% | 0.369% |
| 67 | 13.916 | 1033 | 1035 | 1038 | rVV | 2028379 | 1907696 | 19.98% | 2.510% |
| 68 | 14.099 | 1049 | 1051 | 1053 | rBV | 215898 | 216006 | 2.26% | 0.284% |
| 69 | 14.397 | 1075 | 1077 | 1079 | rVB | 119242 | 150113 | 1.57% | 0.198% |
| 70 | 14.694 | 1101 | 1103 | 1106 | rVB | 202854 | 215971 | 2.26% | 0.284% |
| 71 | 15.014 | 1128 | 1131 | 1133 | rBV | 156766 | 198961 | 2.08% | 0.262% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

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-BF121716.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 72 | 15.322 | 1155 | 1158 | 1160 | rBV | 1172758 | 1481560 | 15.52% | 1.950% |
| 73 | 15.357 | 1160 | 1161 | 1165 | rVB | 149669 | 197249 | 2.07% | 0.260% |
| 74 | 15.757 | 1194 | 1196 | 1201 | rVB | 108635 | 187786 | 1.97% | 0.247% |
| 75 | 16.225 | 1234 | 1237 | 1243 | rVB | 100805 | 194599 | 2.04% | 0.256% |
| 76 | 16.762 | 1282 | 1284 | 1288 | rVB | 66561 | 110369 | 1.16% | 0.145% |
| 77 | 17.391 | 1337 | 1339 | 1344 | rVB3 | 45252 | 114737 | 1.20% | 0.151% |

Sum of corrected areas: 75988863

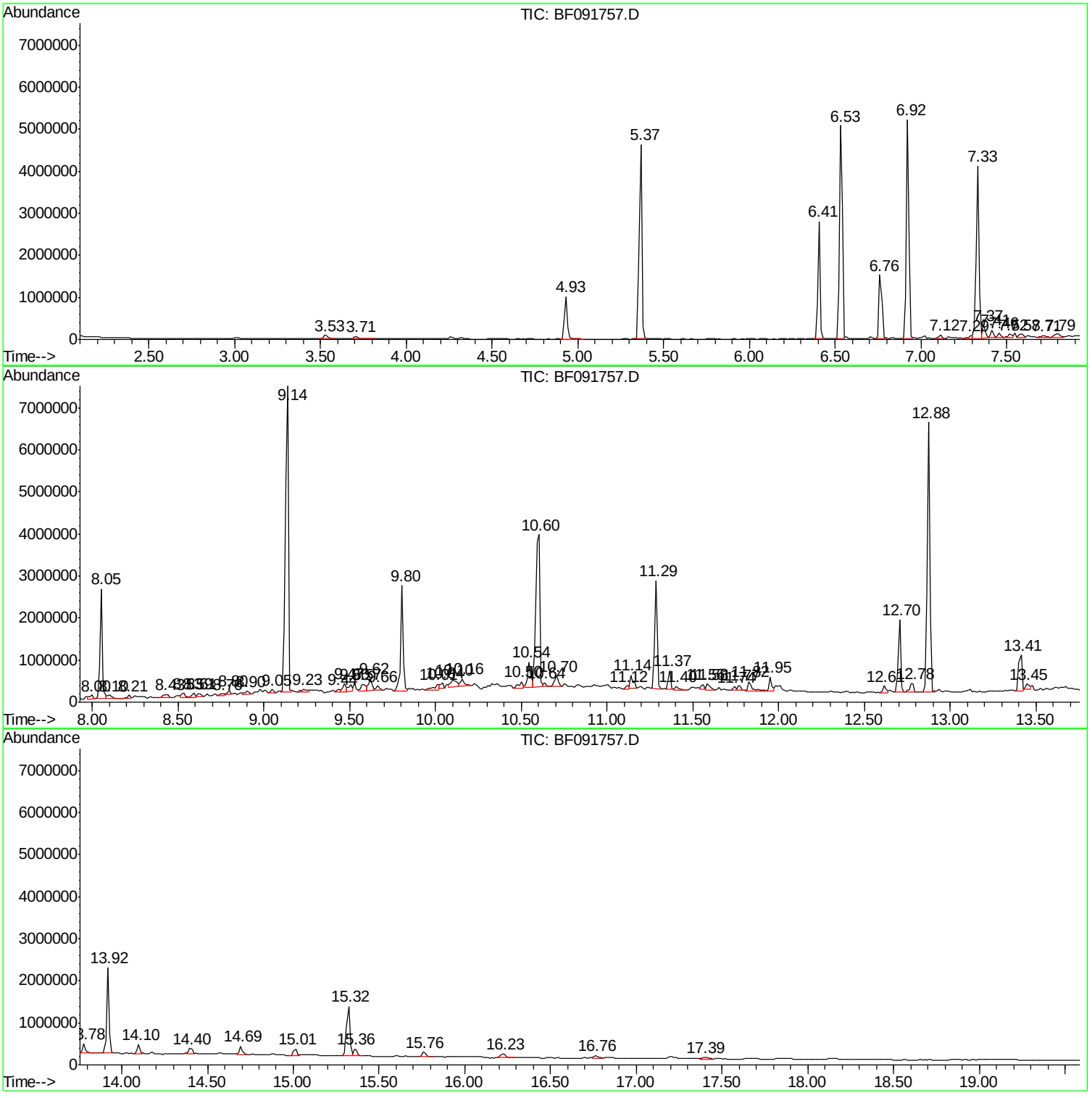
LSC Report - Integrated Chromatogram

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

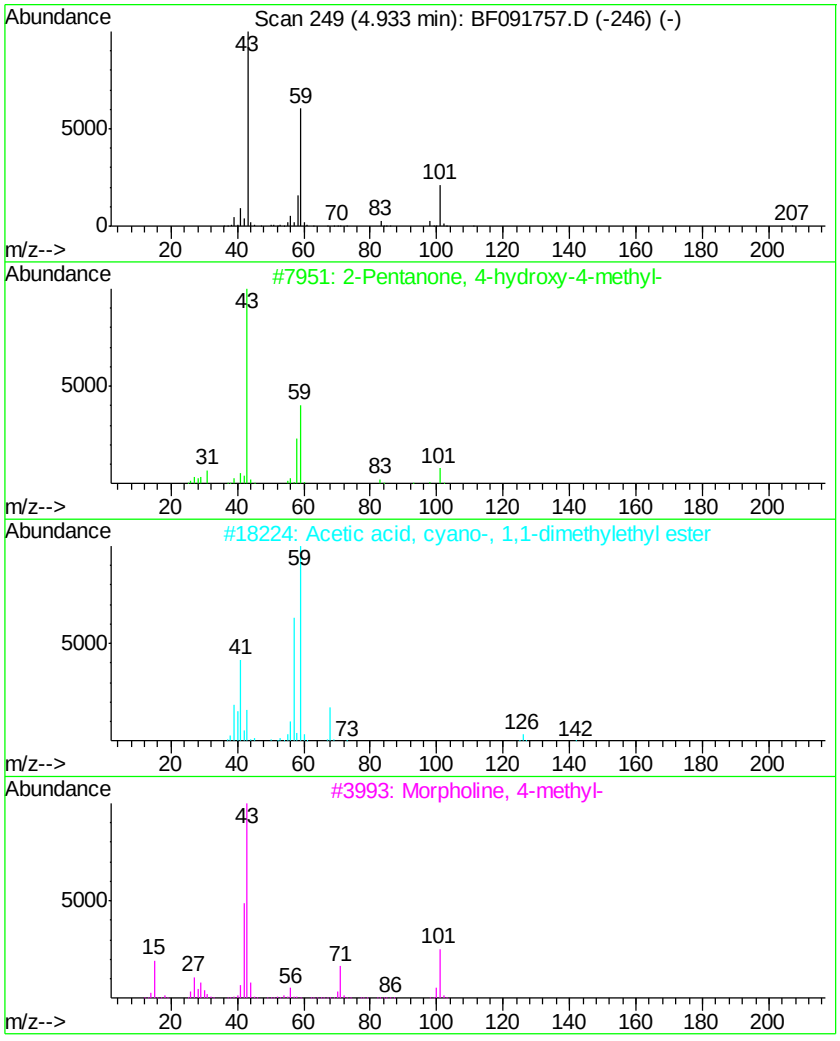
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

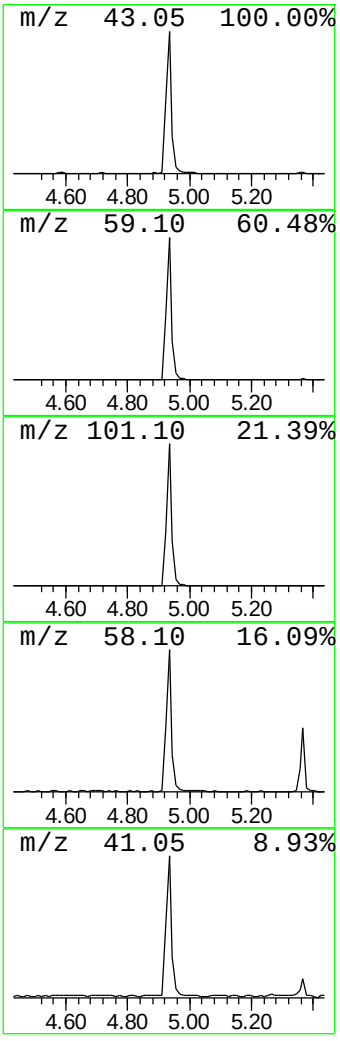
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.93 | 14.86 ng | 1260570 | 1,4-Dichlorobenzene-d4 | 6.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Pentanone, 4-hydroxy-4-methyl- | 116 | C6H12O2 | 000123-42-2 | 56 |
| 2 | Acetic acid, cyano-, 1,1-dimethy... | 141 | C7H11NO2 | 001116-98-9 | 23 |
| 3 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 4 | Butane, 1-ethoxy- | 102 | C6H14O | 000628-81-9 | 9 |
| 5 | 1,3-Dioxolane-2-methanol, 2,4-di... | 132 | C6H12O3 | 053951-43-2 | 9 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

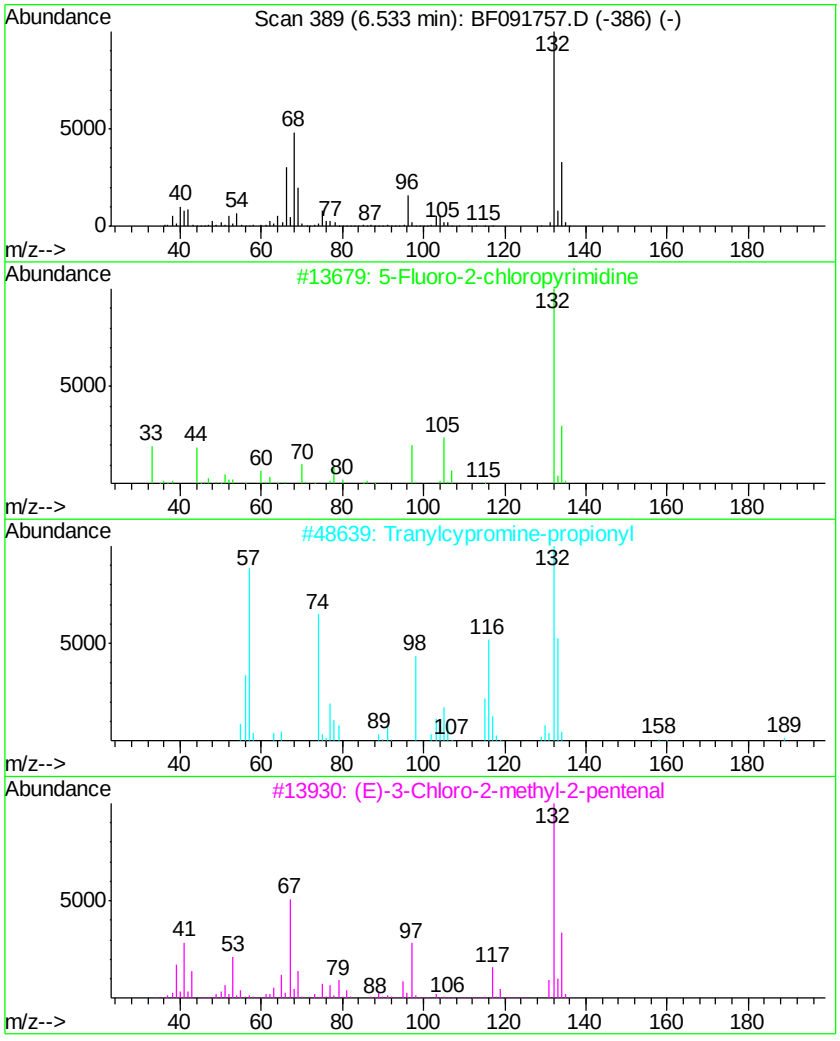
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

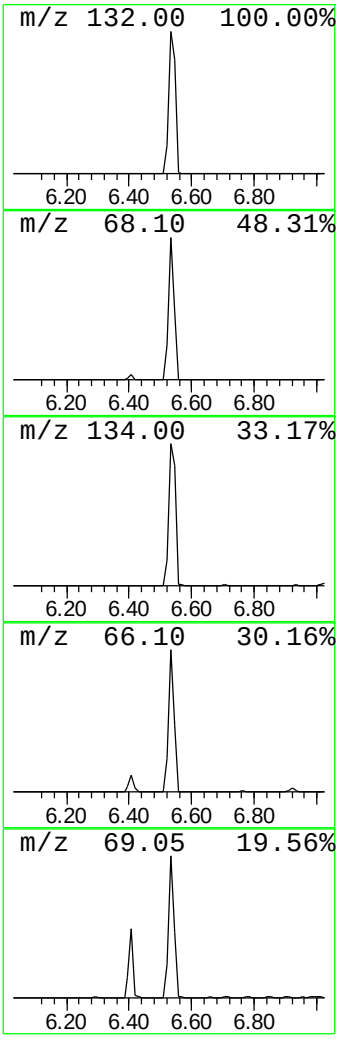
**********

Peak Number 2 unknown6.53 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 6.53 | 75.67 ng | 6417540 | 1,4-Dichlorobenzene-d4 | 6.76 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 16 |
| 2 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 3 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 9 |
| 4 | Bicyclo[4.2.0]octa-1,3,5-triene,... | 132 | C10H12 | 028749-81-7 | 9 |
| 5 | Benzene, 1-ethenyl-3,5-dimethyl- | 132 | C10H12 | 005379-20-4 | 9 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

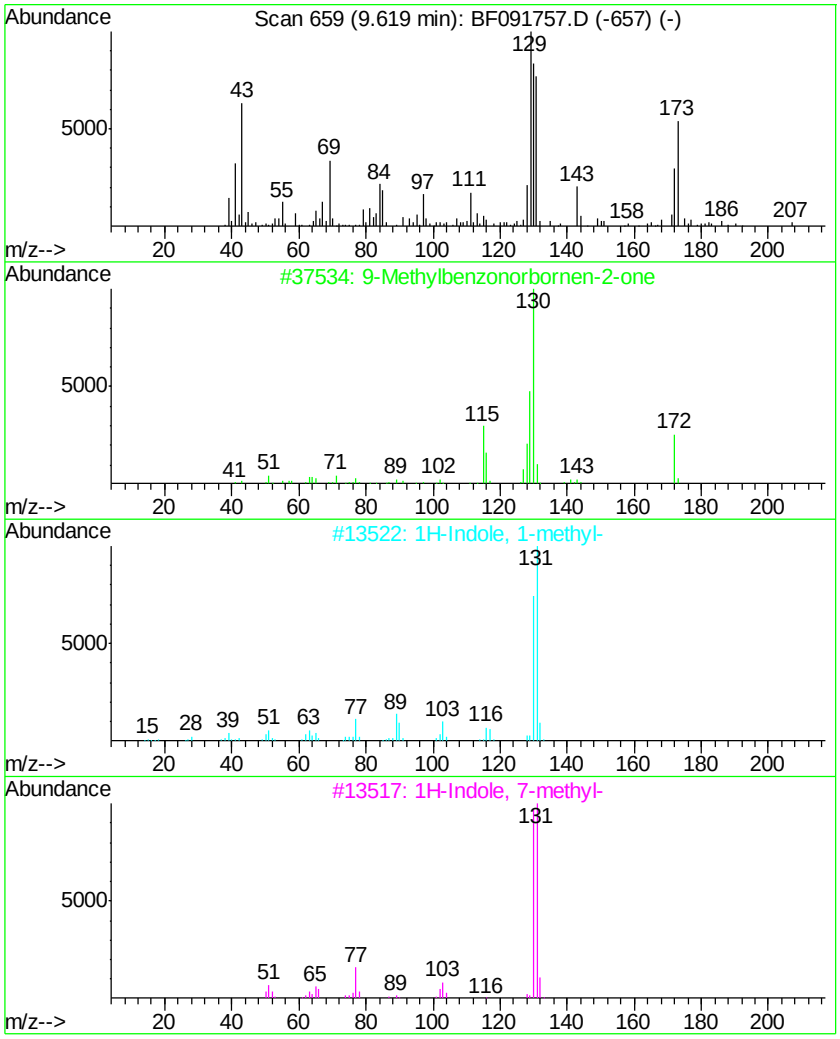
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

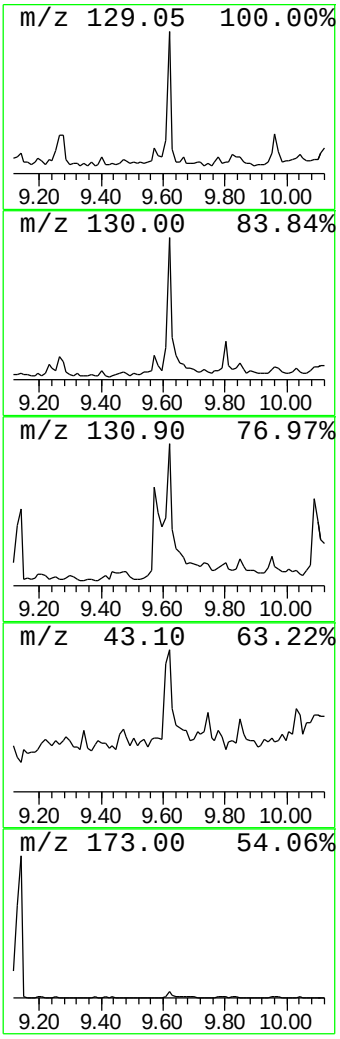
**********

Peak Number 4 unknown9.62 Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 9.62 | 3.32 ng | 429221 | Acenaphthene-d10 | 9.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 9-Methylbenzonorbornen-2-one | 172 | C12H12O | 1000110-51-6 | 35 |
| 2 | 1H-Indole, 1-methyl- | 131 | C9H9N | 000603-76-9 | 27 |
| 3 | 1H-Indole, 7-methyl- | 131 | C9H9N | 000933-67-5 | 27 |
| 4 | 1H-Indole, 4-methyl- | 131 | C9H9N | 016096-32-5 | 27 |
| 5 | 1H-Indole, 6-methyl- | 131 | C9H9N | 003420-02-8 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

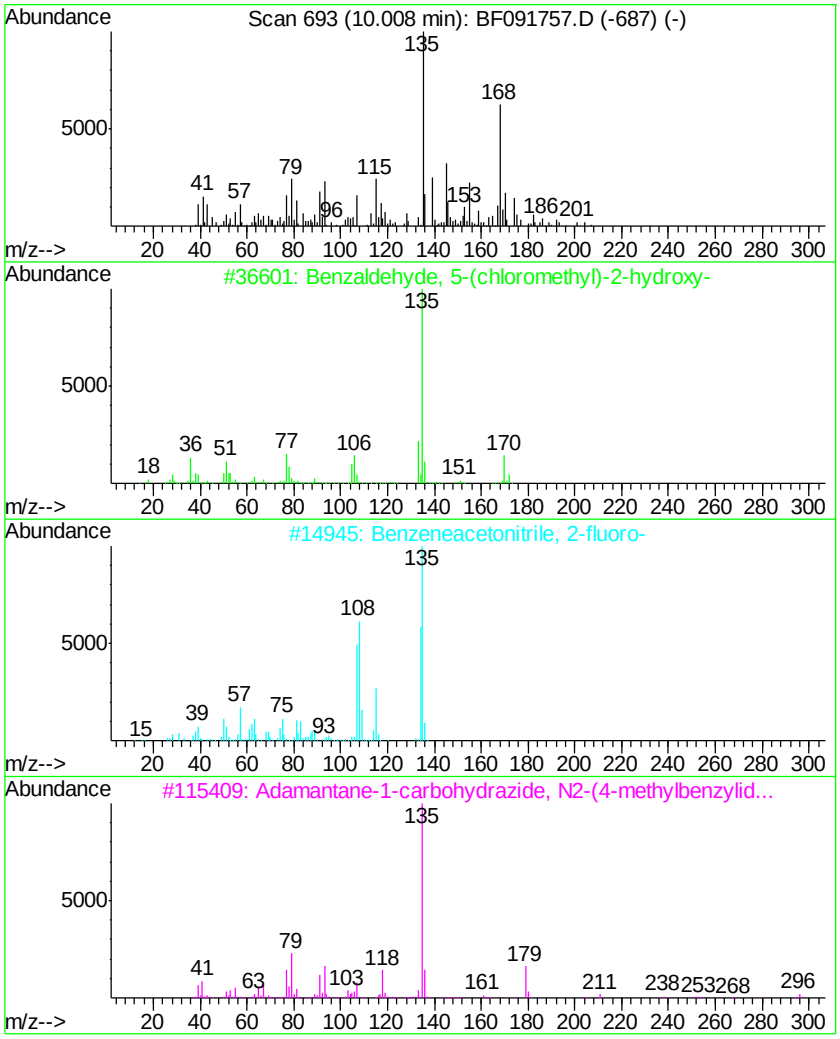
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

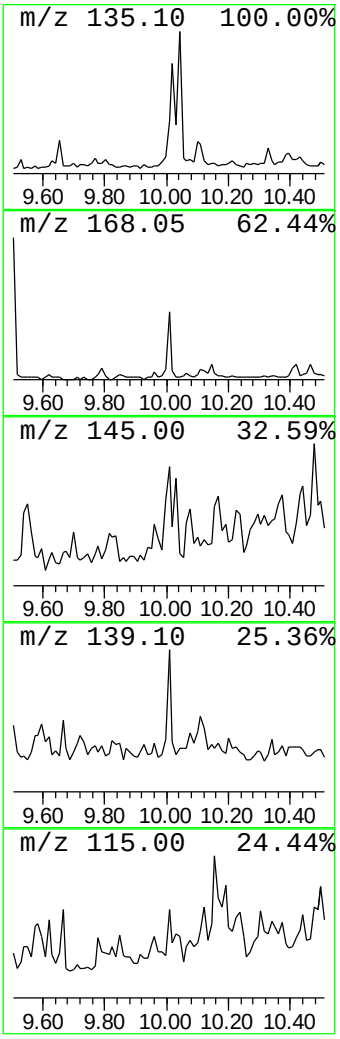
**********

Peak Number 5 unknown10.01 Concentration Rank 17

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.01 | 2.75 ng | 355732 | Acenaphthene-d10 | 9.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzaldehyde, 5-(chloromethyl)-2... | 170 | C8H7ClO2 | 023731-06-8 | 27 |
| 2 | Benzeneacetonitrile, 2-fluoro- | 135 | C8H6FN | 000326-62-5 | 25 |
| 3 | Adamantane-1-carbohydrazide, N2-... | 296 | C19H24N2O | 1000263-64-4 | 25 |
| 4 | Benzeneacetamide, .alpha.-ethyl-... | 207 | C11H13NO3 | 056440-45-0 | 25 |
| 5 | 2-Iodoadamantane | 262 | C10H15I | 018971-91-0 | 25 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

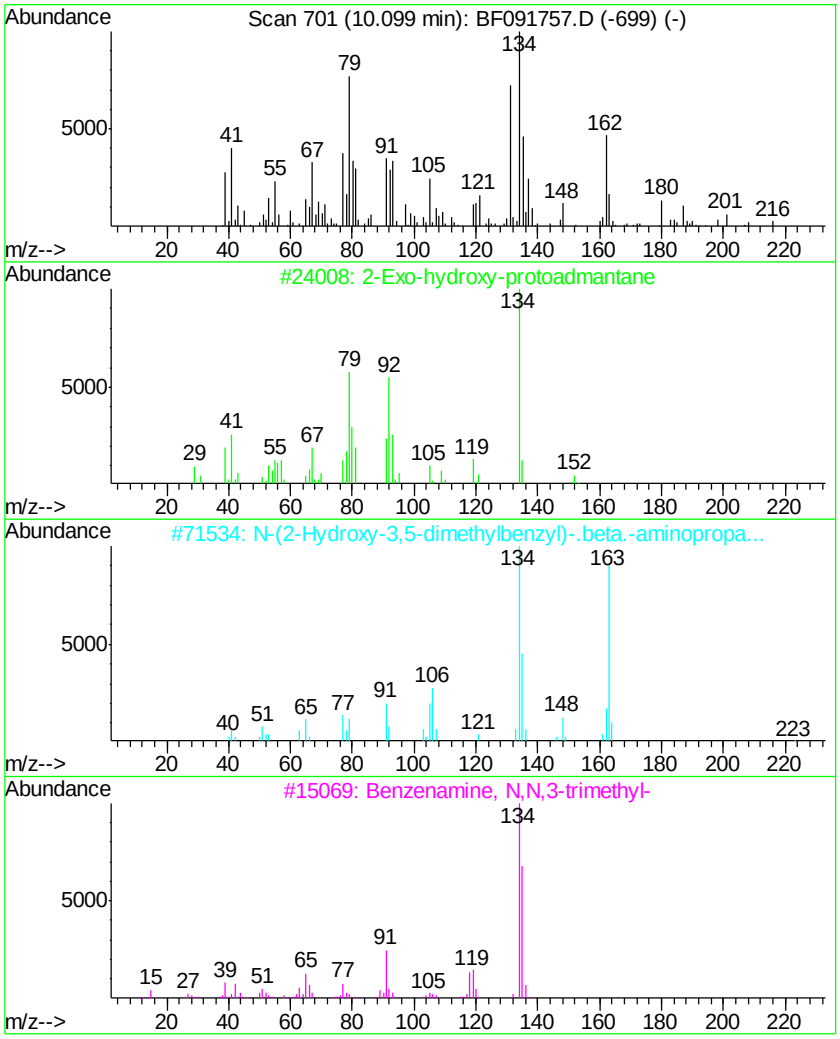
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

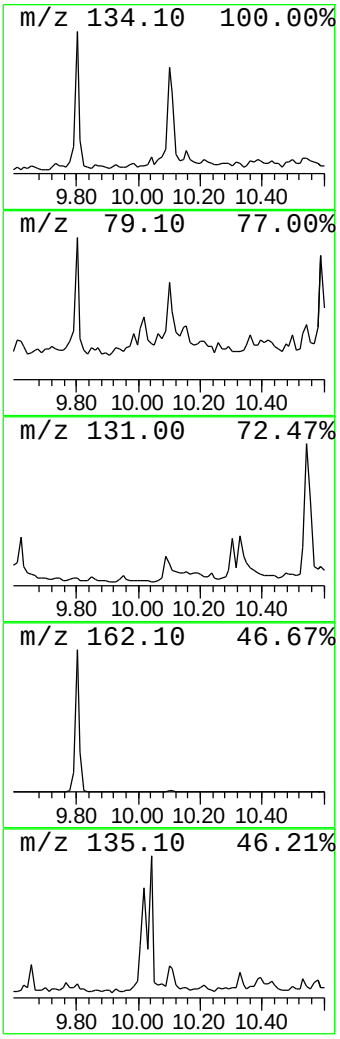
**********

Peak Number 6 unknown10.10 Concentration Rank 14

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.10 | 3.00 ng | 387428 | Acenaphthene-d10 | 9.80 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Exo-hydroxy-protoadmantane | 152 | C10H16O | 1000146-18-8 | 35 |
| 2 | N-(2-Hydroxy-3,5-dimethylbenzyl)... | 223 | C12H17NO3 | 082645-12-3 | 27 |
| 3 | Benzenamine, N,N,3-trimethyl- | 135 | C9H13N | 000121-72-2 | 25 |
| 4 | Benzenamine, N,N,4-trimethyl- | 135 | C9H13N | 000099-97-8 | 25 |
| 5 | Tricyclo[4.4.0.0(2,8)]decane, 3-... | 194 | C12H18O2 | 1000196-68-9 | 22 |



Library Search Compound Report

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

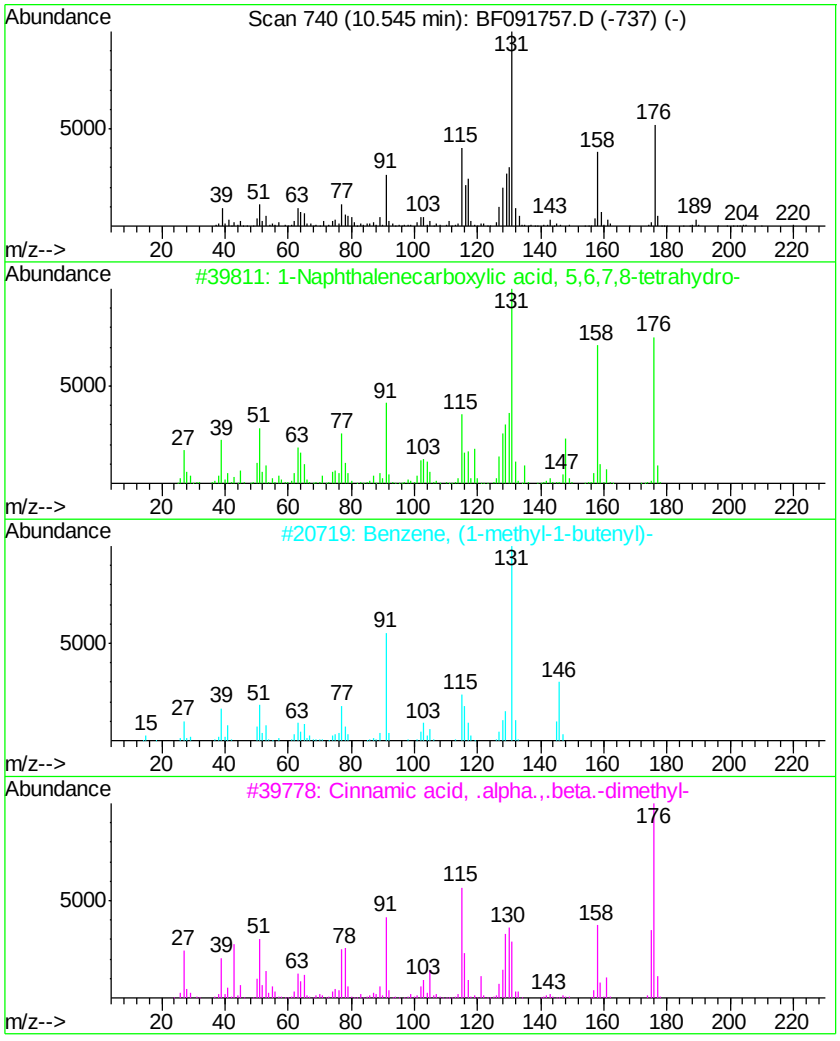
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

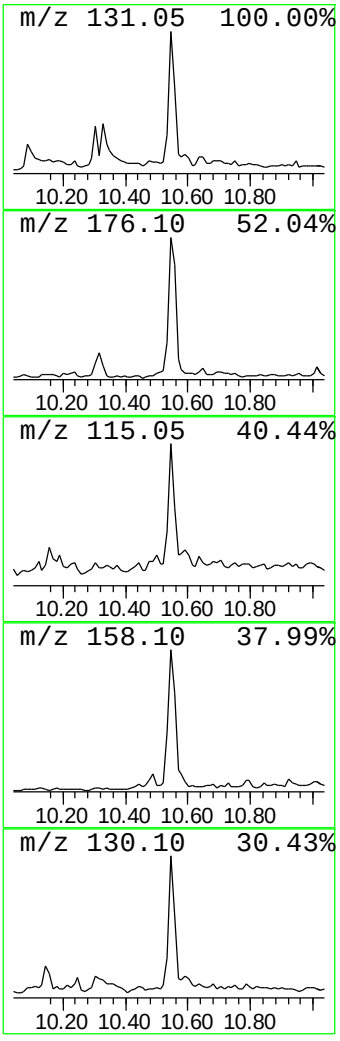
**********

Peak Number 7 1-Naphthalenecarboxylic aci... Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.54 | 7.16 ng | 874536 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Naphthalenecarboxylic acid, 5,... | 176 | C11H12O2 | 004242-18-6 | 81 |
| 2 | Benzene, (1-methyl-1-butenyl)- | 146 | C11H14 | 053172-84-2 | 47 |
| 3 | Cinnamic acid, .alpha.,.beta.-di... | 176 | C11H12O2 | 1000151-56-4 | 47 |
| 4 | 3-Pentenoic acid, 4-phenyl- | 176 | C11H12O2 | 053774-19-9 | 47 |
| 5 | Cyclopropane, 2-bromo-1-methyl-1... | 210 | C10H11Br | 055091-64-0 | 41 |



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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

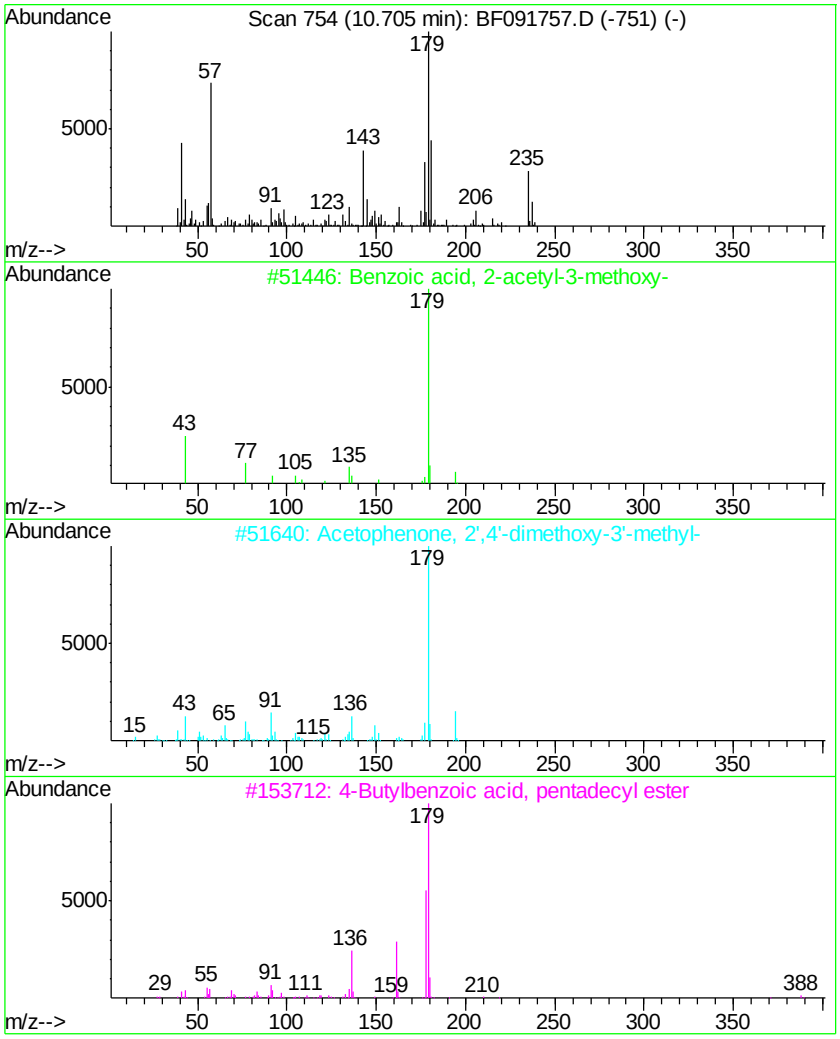
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

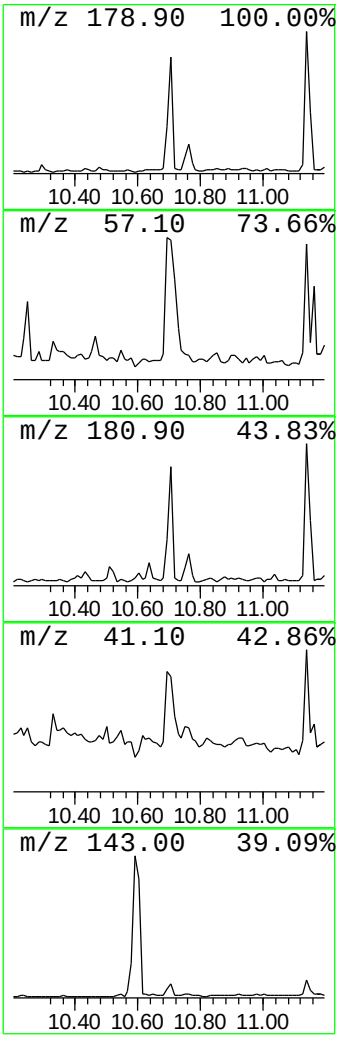
**********

Peak Number 8 unknown10.70 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 10.70 | 3.27 ng | 399040 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Benzoic acid, 2-acetyl-3-methoxy- | 194 | C10H10O4 | 120714-42-3 | 12 |
| 2 | Acetophenone, 2',4'-dimethoxy-3'... | 194 | C11H14O3 | 060512-80-3 | 10 |
| 3 | 4-Butylbenzoic acid, pentadecyl ... | 388 | C26H44O2 | 1000292-32-8 | 10 |
| 4 | 4-Butylbenzoic acid, hexadecyl e... | 402 | C27H46O2 | 1000292-32-9 | 10 |
| 5 | N-Methyl-1-noradamantane carboxa... | 179 | C11H17NO | 1000211-82-0 | 10 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

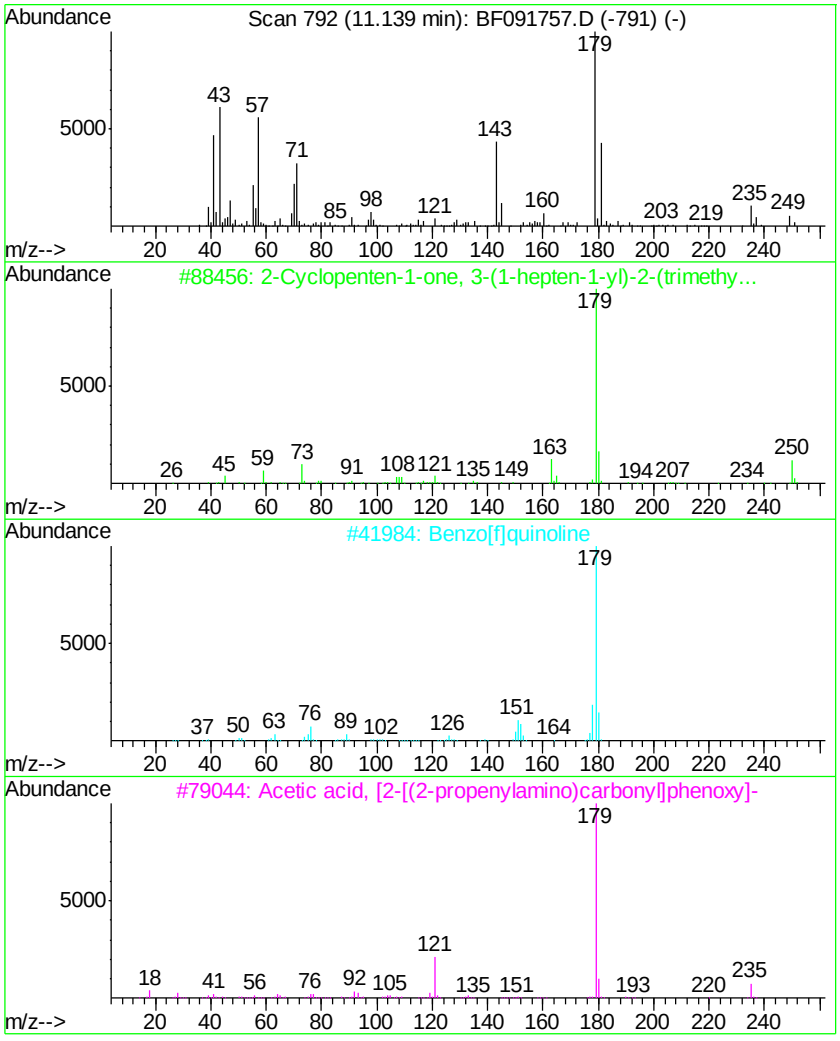
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

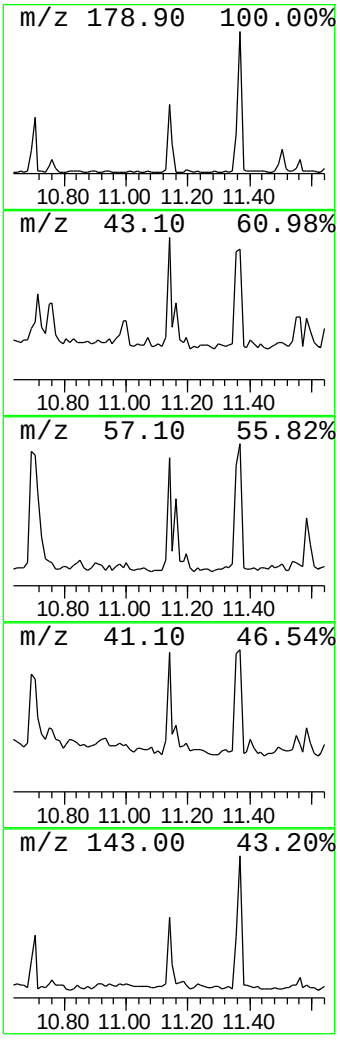
**********

Peak Number 9 unknown11.14 Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.14 | 3.35 ng | 409082 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Cyclopenten-1-one, 3-(1-hepten... | 250 | C15H26OSi | 1000159-28-7 | 10 |
| 2 | Benzo[f]quinoline | 179 | C13H9N | 000085-02-9 | 9 |
| 3 | Acetic acid, [2-[(2-propenylamin... | 235 | C12H13NO4 | 000119-45-9 | 9 |
| 4 | 4-tert-Butyl-2-nitroacetanilide | 236 | C12H16N2O3 | 040655-37-6 | 9 |
| 5 | 1,2-Dimethylpropyl trifluoroacetate | 184 | C7H11F3O2 | 000691-75-8 | 9 |



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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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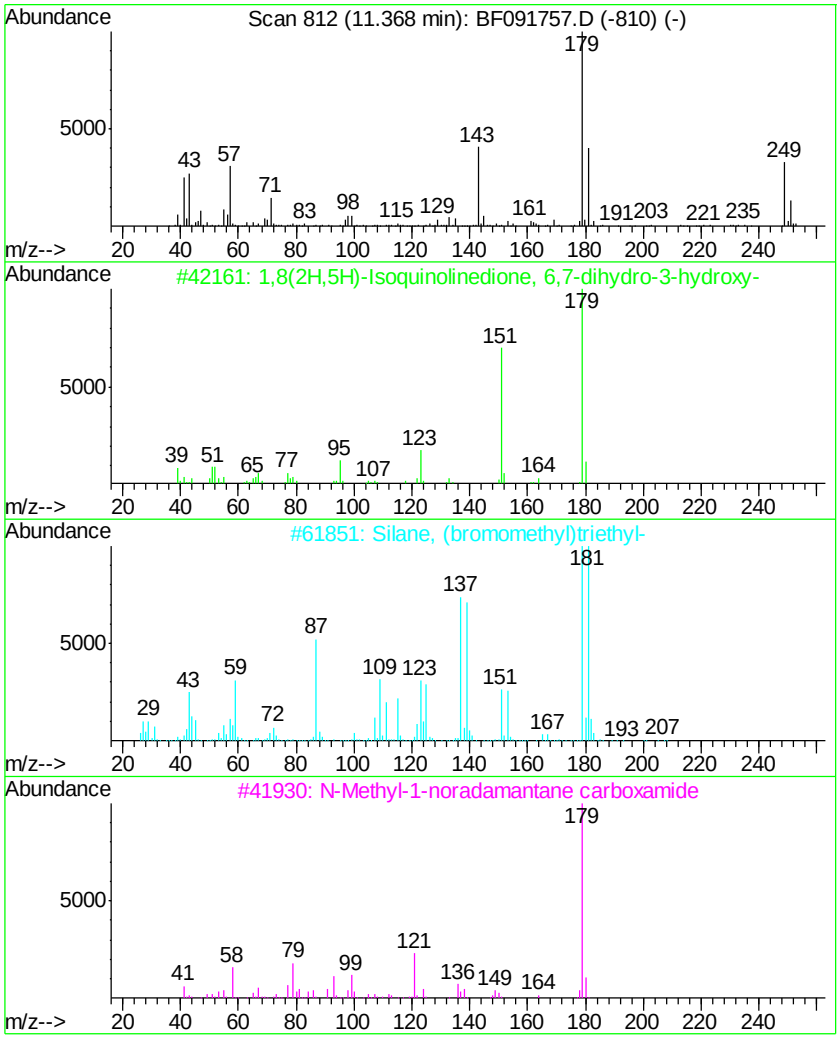
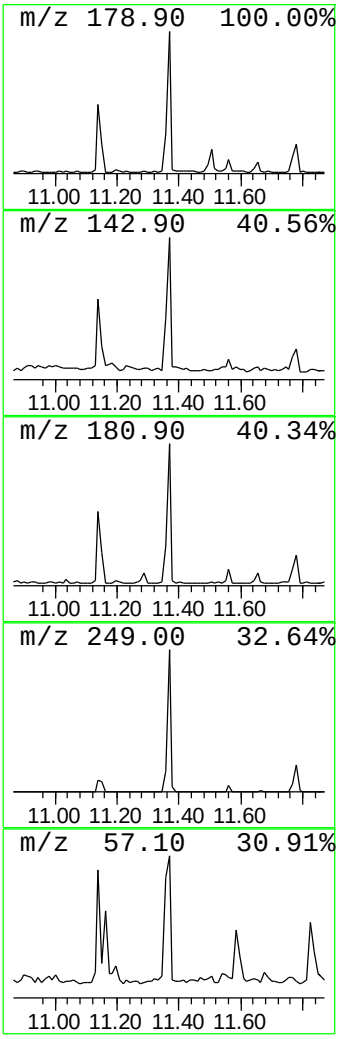
Peak Number 10 unknown11.37 Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.37 | 3.87 ng | 473133 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,8(2H,5H)-Isoquinolinedione, 6,... | 179 | C9H9NO3 | 037704-54-4 | 10 |
| 2 | Silane, (bromomethyl)triethyl- | 208 | C7H17BrSi | 001112-53-4 | 10 |
| 3 | N-Methyl-1-noradamantane carboxa... | 179 | C11H17NO | 1000211-82-0 | 9 |
| 4 | [1,1'-Biphenyl]-2-carbonitrile | 179 | C13H9N | 024973-49-7 | 9 |
| 5 | Benzo[f]isoquinoline | 179 | C13H9N | 000229-67-4 | 9 |



# Library Search Compound Report

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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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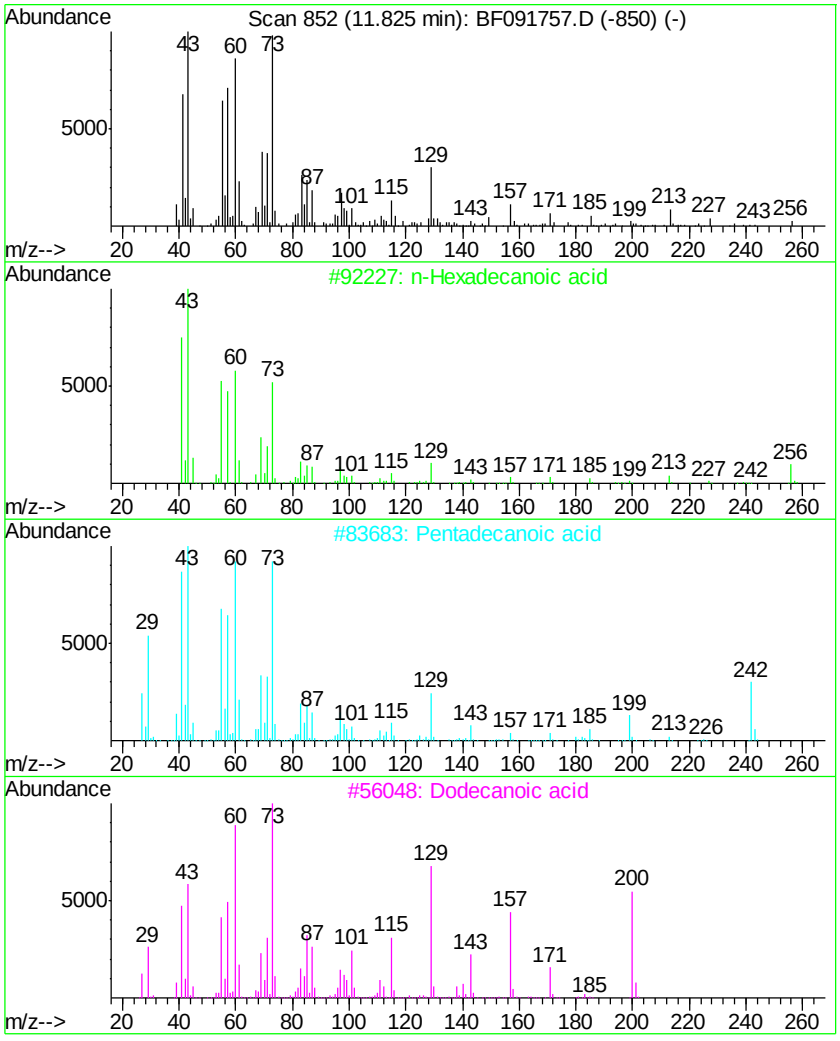
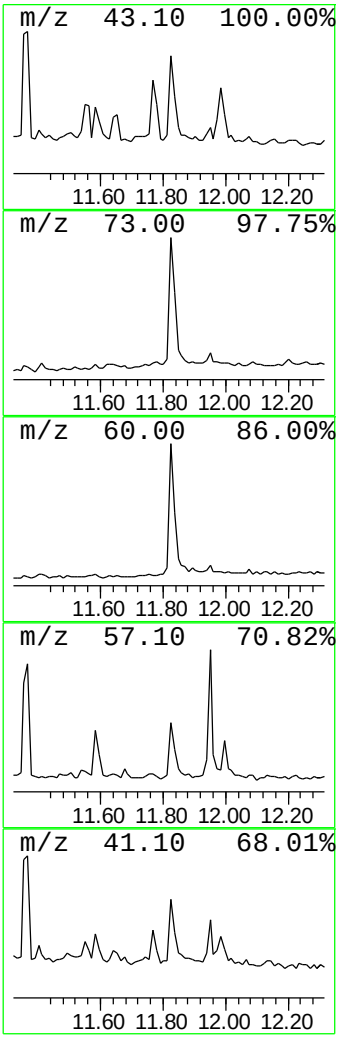
Peak Number 11 n-Hexadecanoic acid Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.82 | 3.17 ng | 387291 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 91 |
| 2 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 87 |
| 3 | Dodecanoic acid | 200 | C12H24O2 | 000143-07-7 | 87 |
| 4 | Undecanoic acid | 186 | C11H22O2 | 000112-37-8 | 78 |
| 5 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |



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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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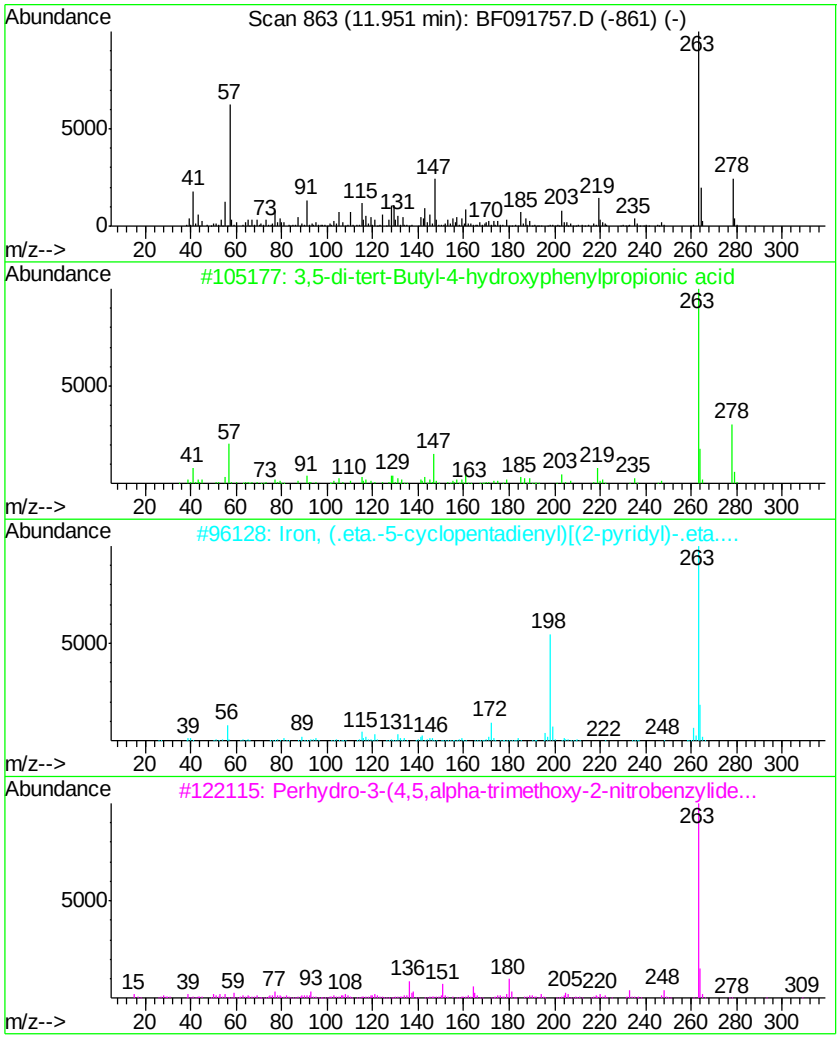
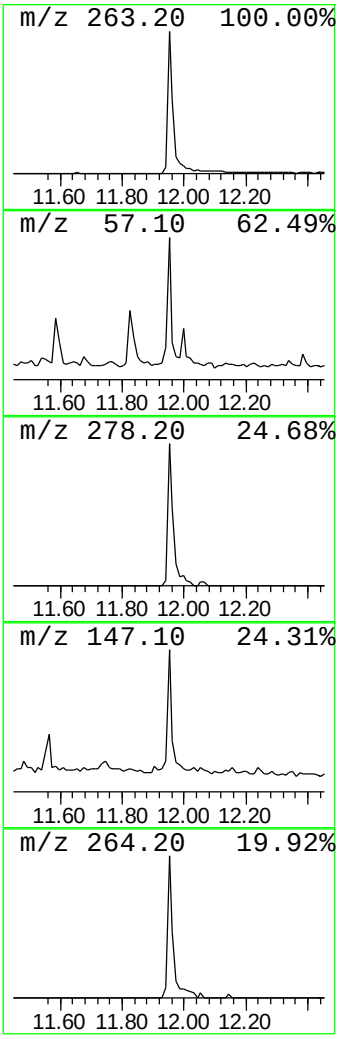
Peak Number 12 3,5-di-tert-Butyl-4-hydroxy... Concentration Rank 13

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 11.95 | 3.02 ng | 368353 | Phenanthrene-d10 | 11.29 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3,5-di-tert-Butyl-4-hydroxyphenyl... | 278 | C17H26O3 | 020170-32-5 | 94 |
| 2 | Iron, (.eta.-5-cyclopentadienyl)... | 263 | C15H13FeN | 1000164-28-2 | 46 |
| 3 | Perhydro-3-(4,5,alpha-trimethoxy... | 309 | C14H15NO7 | 093005-00-6 | 43 |
| 4 | Trimethyl(2,6 ditert.-butylpheno... | 278 | C17H30OSi | 010416-73-6 | 40 |
| 5 | Quinoline-4-carboxylic acid, 2-(... | 263 | C17H13NO2 | 020389-05-3 | 38 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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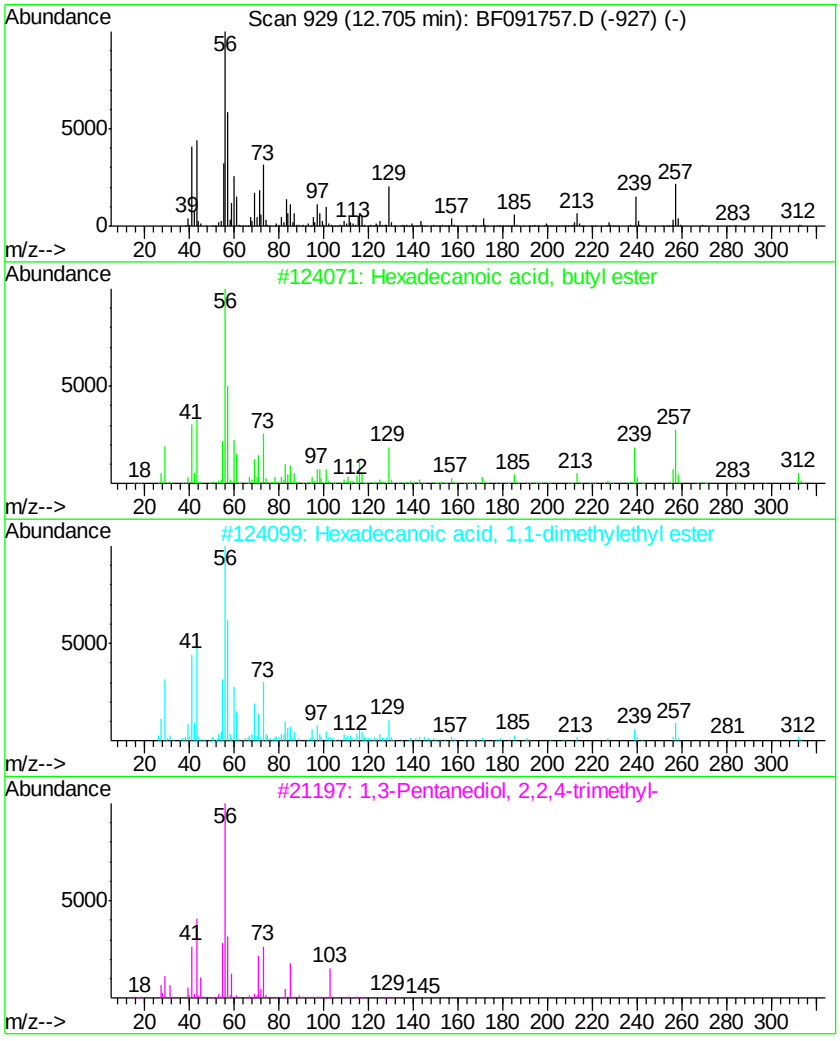
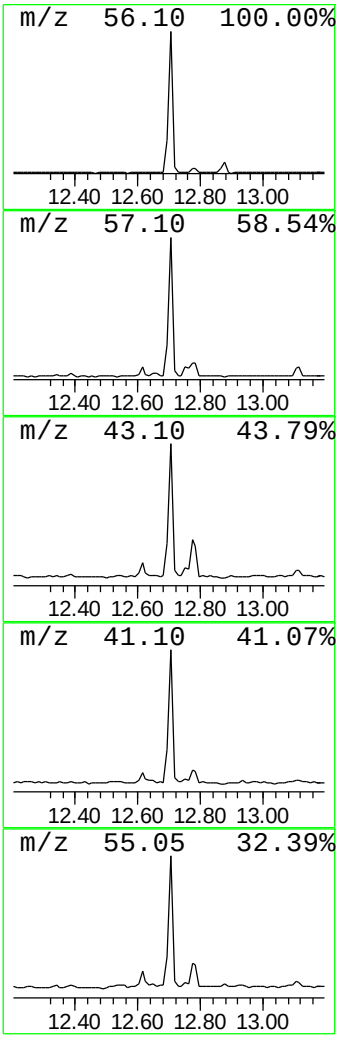
Peak Number 13 Hexadecanoic acid, butyl ester Concentration Rank 3

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.70 | 15.52 ng | 1480670 | Chrysene-d12 | 13.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Hexadecanoic acid, butyl ester | 312 | C20H40O2 | 000111-06-8 | 91 |
| 2 | Hexadecanoic acid, 1,1-dimethyle... | 312 | C20H40O2 | 031158-91-5 | 74 |
| 3 | 1,3-Pentanediol, 2,2,4-trimethyl- | 146 | C8H18O2 | 000144-19-4 | 38 |
| 4 | 1,3-Hexanediol, 2-ethyl- | 146 | C8H18O2 | 000094-96-2 | 35 |
| 5 | Cyclobutane, 1,1-dimethyl-2-octyl- | 196 | C14H28 | 062338-30-1 | 35 |



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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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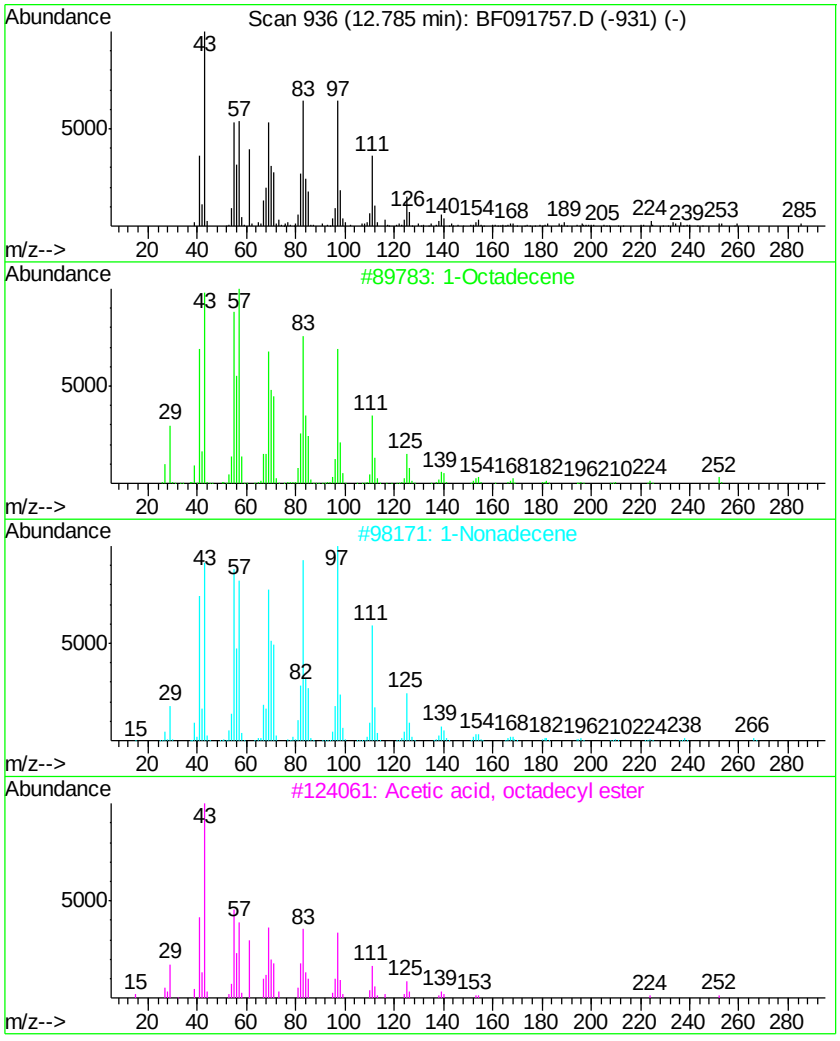
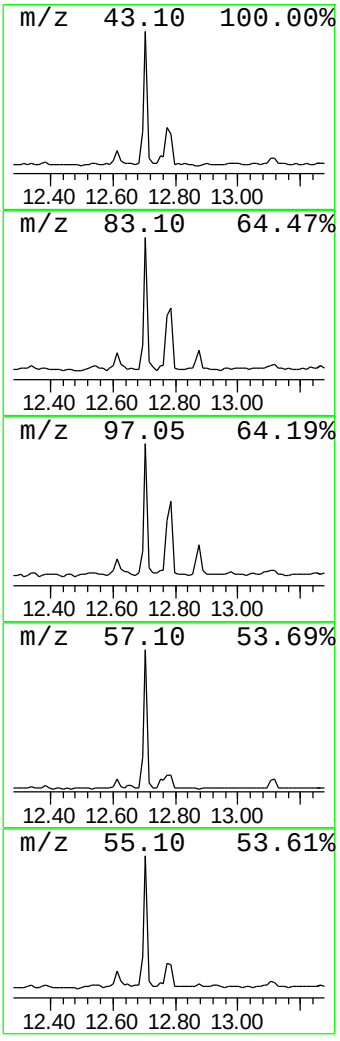
Peak Number 14 1-Octadecene Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 12.78 | 3.90 ng | 371606 | Chrysene-d12 | 13.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Octadecene | 252 | C18H36 | 000112-88-9 | 94 |
| 2 | 1-Nonadecene | 266 | C19H38 | 018435-45-5 | 93 |
| 3 | Acetic acid, octadecyl ester | 312 | C20H40O2 | 000822-23-1 | 91 |
| 4 | 1-Hexadecene | 224 | C16H32 | 000629-73-2 | 90 |
| 5 | 1-Heptadecanol, acetate | 298 | C19H38O2 | 000822-20-8 | 87 |



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Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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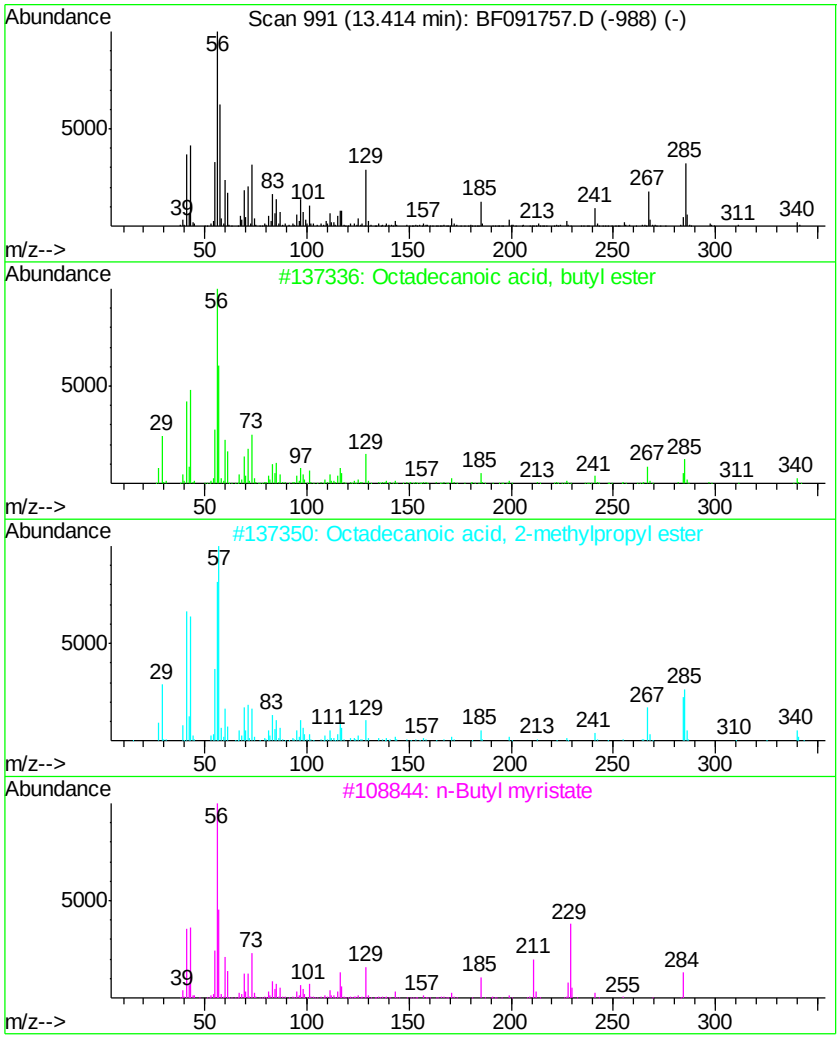
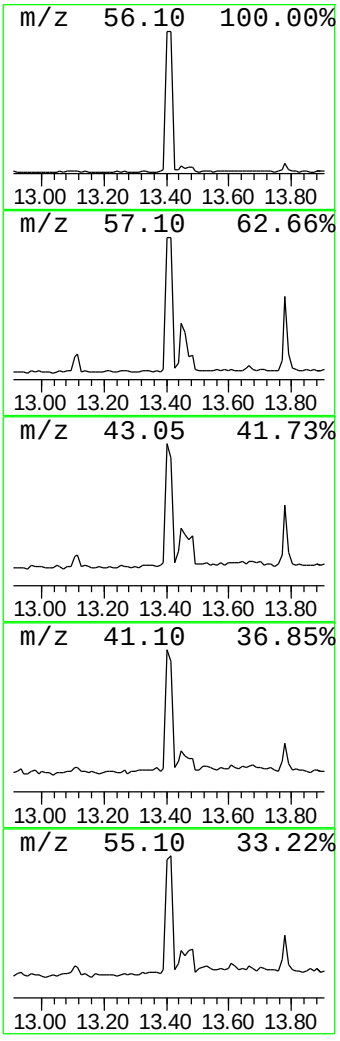
Peak Number 15 Octadecanoic acid, butyl ester Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.41 | 11.20 ng | 1068200 | Chrysene-d12 | 13.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecanoic acid, butyl ester | 340 | C22H44O2 | 000123-95-5 | 96 |
| 2 | Octadecanoic acid, 2-methylpropy... | 340 | C22H44O2 | 000646-13-9 | 80 |
| 3 | n-Butyl myristate | 284 | C18H36O2 | 000110-36-1 | 52 |
| 4 | 1-Pentene, 2,4-dimethyl- | 98 | C7H14 | 002213-32-3 | 27 |
| 5 | 2-Methyl-1-octadecene | 266 | C19H38 | 061868-20-0 | 27 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

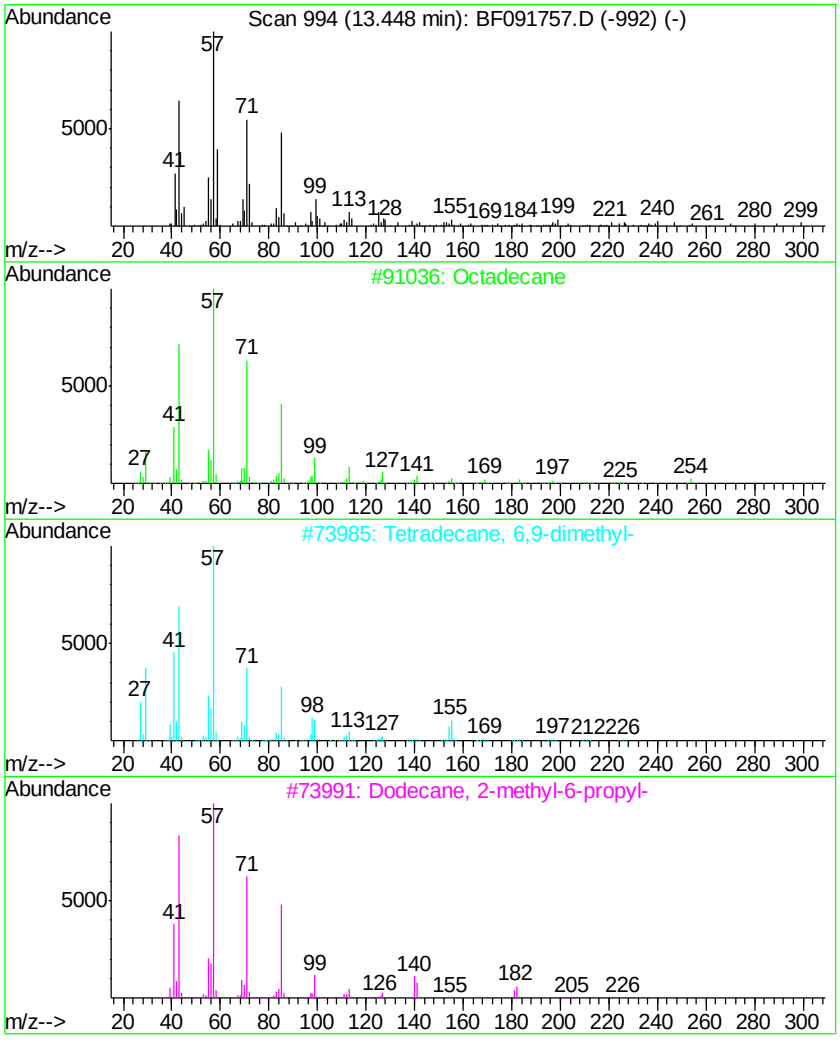
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

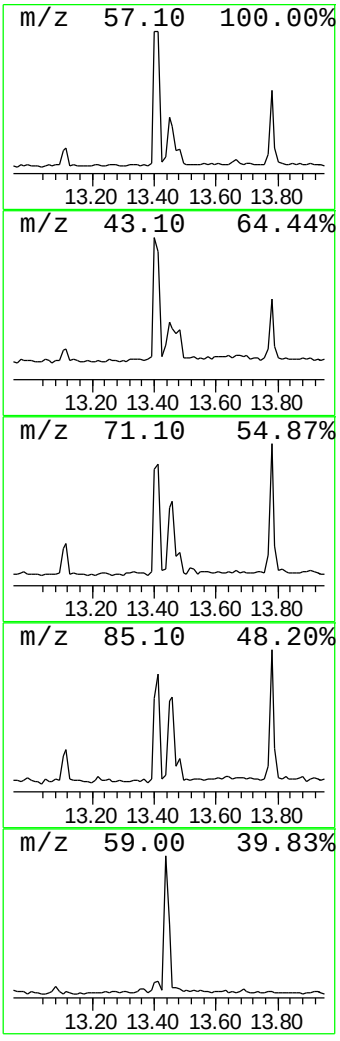
**********

Peak Number 16 Octadecane Concentration Rank 20

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.45 | 2.54 ng | 242119 | Chrysene-d12 | 13.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octadecane | 254 | C18H38 | 000593-45-3 | 50 |
| 2 | Tetradecane, 6,9-dimethyl- | 226 | C16H34 | 055045-13-1 | 49 |
| 3 | Dodecane, 2-methyl-6-propyl- | 226 | C16H34 | 055045-08-4 | 49 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 49 |
| 5 | Heptadecane | 240 | C17H36 | 000629-78-7 | 49 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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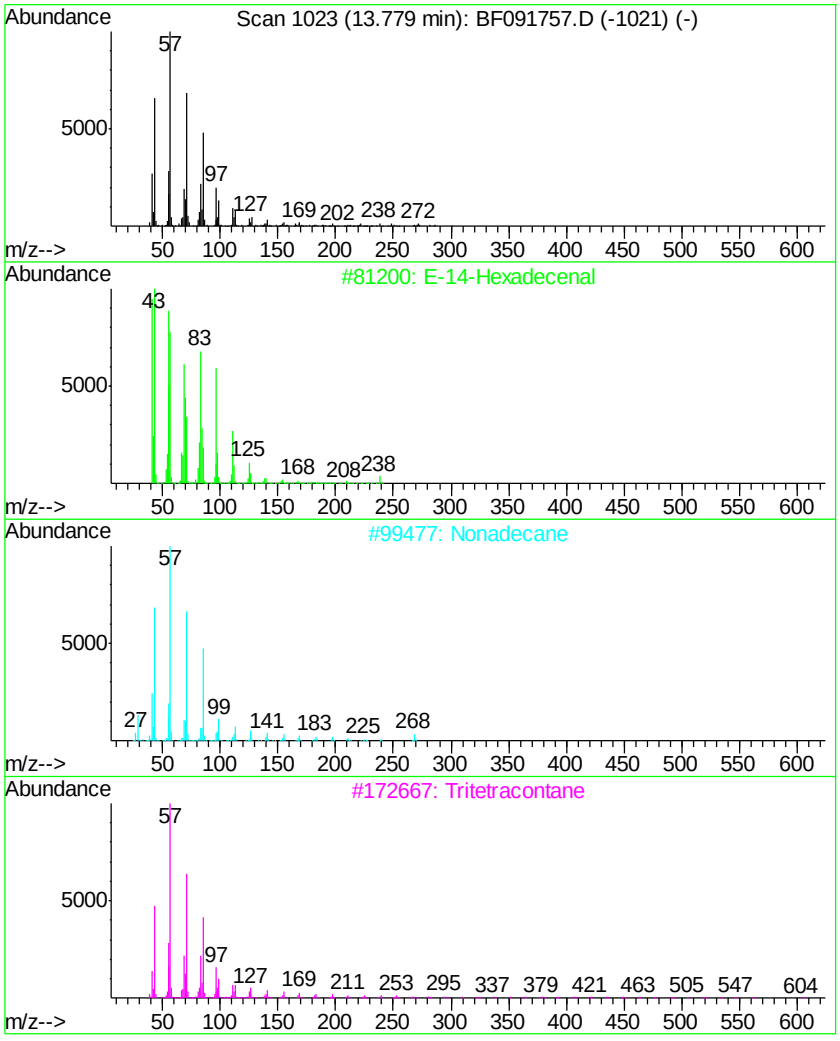
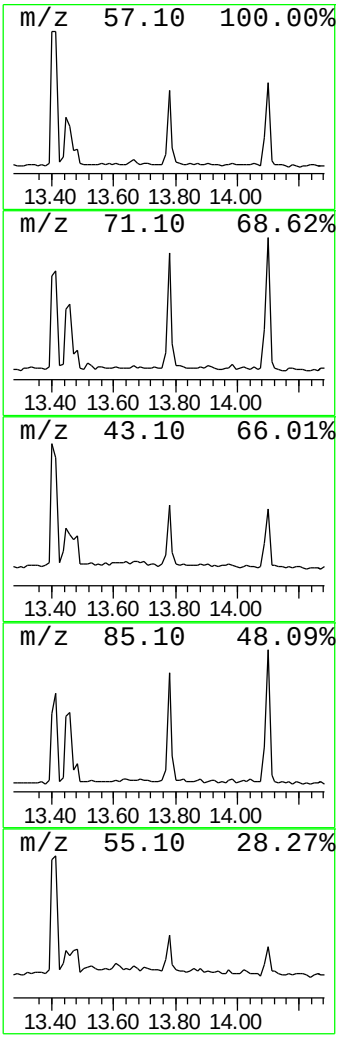
Peak Number 17 E-14-Hexadecenal Concentration Rank 15

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 13.78 | 2.94 ng | 280035 | Chrysene-d12 | 13.92 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | E-14-Hexadecenal | 238 | C16H30O | 330207-53-9 | 93 |
| 2 | Nonadecane | 268 | C19H40 | 000629-92-5 | 91 |
| 3 | Tritetracontane | 605 | C43H88 | 007098-21-7 | 91 |
| 4 | Heptacosane, 1-chloro- | 414 | C27H55Cl | 062016-79-9 | 91 |
| 5 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 87 |



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Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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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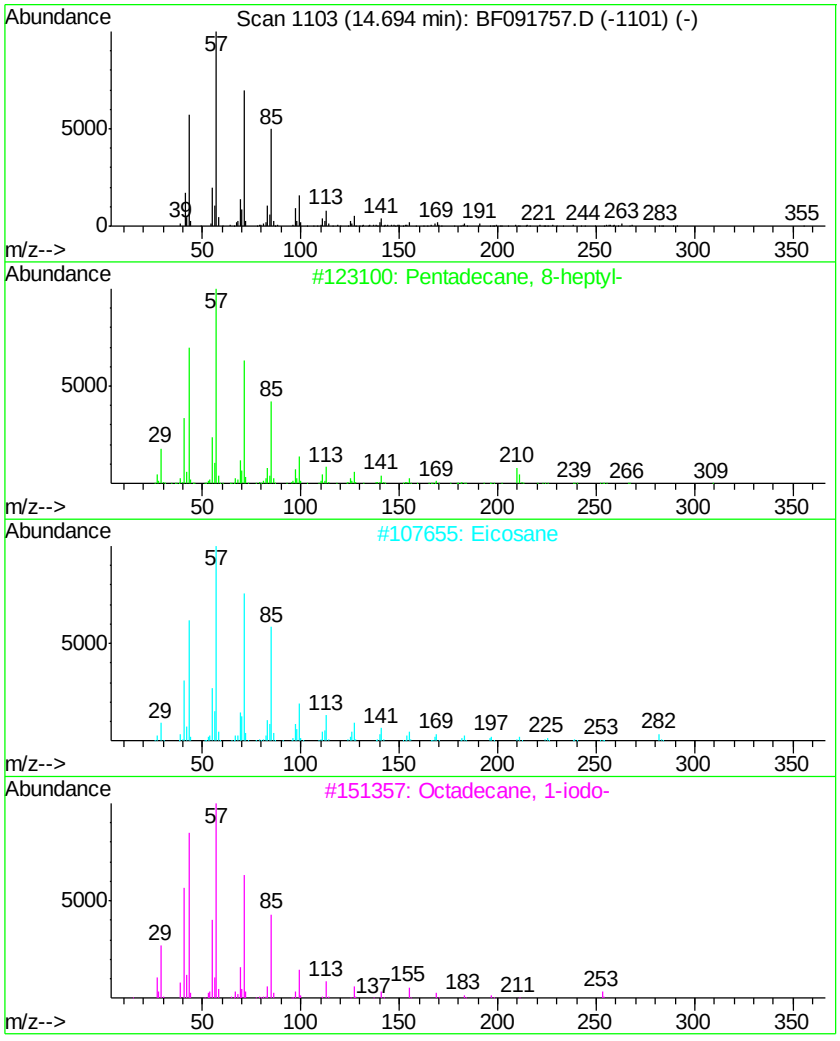
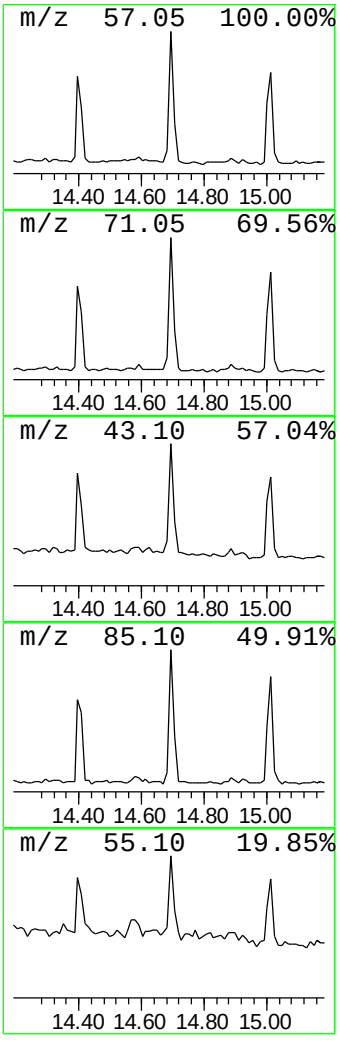
Peak Number 18 Pentadecane, 8-heptyl- Concentration Rank 16

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 14.69 | 2.92 ng | 215971 | Perylene-d12 | 15.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 91 |
| 2 | Eicosane | 282 | C20H42 | 000112-95-8 | 91 |
| 3 | Octadecane, 1-iodo- | 380 | C18H37I | 000629-93-6 | 86 |
| 4 | Hexadecane | 226 | C16H34 | 000544-76-3 | 86 |
| 5 | Heptacosane | 380 | C27H56 | 000593-49-7 | 74 |



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

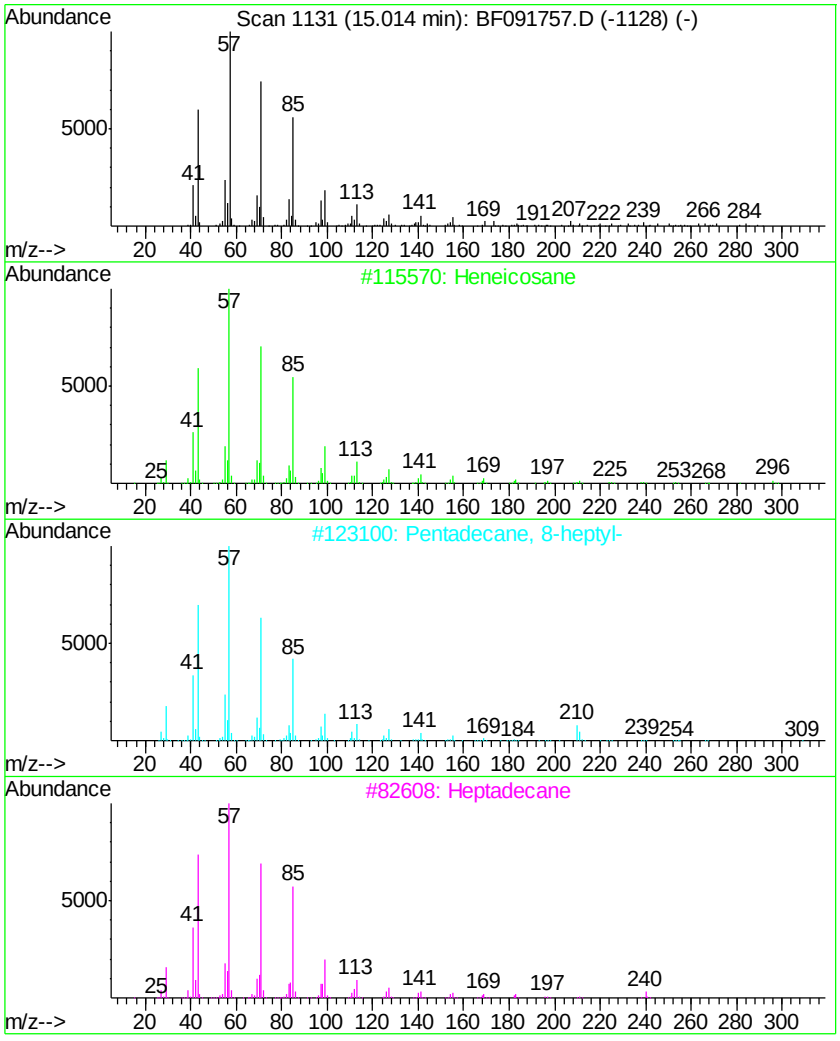
TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

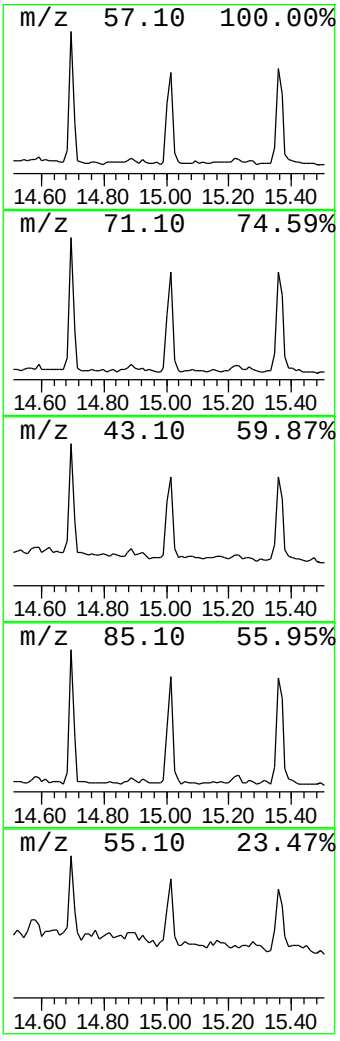
**********

Peak Number 19 Heneicosane Concentration Rank 18

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.01 | 2.69 ng | 198961 | Perylene-d12 | 15.32 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Heneicosane | 296 | C21H44 | 000629-94-7 | 91 |
| 2 | Pentadecane, 8-heptyl- | 310 | C22H46 | 071005-15-7 | 91 |
| 3 | Heptadecane | 240 | C17H36 | 000629-78-7 | 87 |
| 4 | Nonadecane | 268 | C19H40 | 000629-92-5 | 86 |
| 5 | Octadecane | 254 | C18H38 | 000593-45-3 | 80 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121816\
Data File : BF091757.D
Acq On : 19 Dec 2016 00:48
Operator : UM/SJ
Sample : H6091-05
Misc :
ALS Vial : 46 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** MW-36

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF121716.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 |
| 2-Pentanone, 4-hy... | 4.93 | 14.9 | ng | 1260570 | 1 | 6.76 | 1696130 | 20.0 |
| unknown6.53 | 6.53 | 75.7 | ng | 6417540 | 1 | 6.76 | 1696130 | 20.0 |
| unknown9.62 | 9.62 | 3.3 | ng | 429221 | 3 | 9.80 | 2586440 | 20.0 |
| unknown10.01 | 10.01 | 2.8 | ng | 355732 | 3 | 9.80 | 2586440 | 20.0 |
| unknown10.10 | 10.10 | 3.0 | ng | 387428 | 3 | 9.80 | 2586440 | 20.0 |
| 1-Naphthalenecarb... | 10.54 | 7.2 | ng | 874536 | 4 | 11.29 | 2443350 | 20.0 |
| unknown10.70 | 10.70 | 3.3 | ng | 399040 | 4 | 11.29 | 2443350 | 20.0 |
| unknown11.14 | 11.14 | 3.4 | ng | 409082 | 4 | 11.29 | 2443350 | 20.0 |
| unknown11.37 | 11.37 | 3.9 | ng | 473133 | 4 | 11.29 | 2443350 | 20.0 |
| n-Hexadecanoic acid | 11.82 | 3.2 | ng | 387291 | 4 | 11.29 | 2443350 | 20.0 |
| 3,5-di-tert-Butyl... | 11.95 | 3.0 | ng | 368353 | 4 | 11.29 | 2443350 | 20.0 |
| Hexadecanoic acid... | 12.70 | 15.5 | ng | 1480670 | 5 | 13.92 | 1907700 | 20.0 |
| 1-Octadecene | 12.78 | 3.9 | ng | 371606 | 5 | 13.92 | 1907700 | 20.0 |
| Octadecanoic acid... | 13.41 | 11.2 | ng | 1068200 | 5 | 13.92 | 1907700 | 20.0 |
| Octadecane | 13.45 | 2.5 | ng | 242119 | 5 | 13.92 | 1907700 | 20.0 |
| E-14-Hexadecenal | 13.78 | 2.9 | ng | 280035 | 5 | 13.92 | 1907700 | 20.0 |
| Pentadecane, 8-he... | 14.69 | 2.9 | ng | 215971 | 6 | 15.32 | 1481560 | 20.0 |
| Heneicosane | 15.01 | 2.7 | ng | 198961 | 6 | 15.32 | 1481560 | 20.0 |