LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

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-BF060517.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 | 1.602 | 8 | 11 | 33 | rBV | 822361 | 1585438 | 50.48% | 5.880% |
| 2 | 4.619 | 519 | 524 | 546 | rBV | 135172 | 413355 | 13.16% | 1.533% |
| 3 | 5.301 | 635 | 640 | 675 | rBV | 1684307 | 2854297 | 90.89% | 10.586% |
| 4 | 6.960 | 916 | 922 | 933 | rBV | 1626947 | 2574210 | 81.97% | 9.548% |
| 5 | 7.054 | 933 | 938 | 948 | rVB | 1945828 | 2807026 | 89.38% | 10.411% |
| 6 | 7.395 | 992 | 996 | 1013 | rBB | 366589 | 489456 | 15.59% | 1.815% |
| 7 | 7.636 | 1031 | 1037 | 1054 | rBV | 1619176 | 2077010 | 66.14% | 7.703% |
| 8 | 8.313 | 1146 | 1152 | 1176 | rBV | 1138947 | 1661608 | 52.91% | 6.163% |
| 9 | 9.425 | 1337 | 1341 | 1354 | rBV | 613137 | 785374 | 25.01% | 2.913% |
| 10 | 11.213 | 1637 | 1645 | 1656 | rBV | 2355806 | 3140425 | 100.00% | 11.648% |
| 11 | 11.901 | 1756 | 1762 | 1769 | rBV | 380060 | 462443 | 14.73% | 1.715% |
| 12 | 12.248 | 1815 | 1821 | 1827 | rBV2 | 585780 | 706757 | 22.51% | 2.621% |
| 13 | 13.542 | 2036 | 2041 | 2049 | rBV | 1187404 | 1620514 | 51.60% | 6.010% |
| 14 | 13.877 | 2094 | 2098 | 2108 | rVB | 32405 | 45300 | 1.44% | 0.168% |
| 15 | 14.636 | 2224 | 2227 | 2236 | rVB2 | 573255 | 733597 | 23.36% | 2.721% |
| 16 | 15.654 | 2394 | 2400 | 2409 | rBV | 127077 | 165844 | 5.28% | 0.615% |
| 17 | 16.753 | 2583 | 2587 | 2595 | rBV3 | 34061 | 54006 | 1.72% | 0.200% |
| 18 | 17.012 | 2625 | 2631 | 2635 | rVB | 1898399 | 2219467 | 70.67% | 8.232% |
| 19 | 18.265 | 2840 | 2844 | 2851 | rBV | 93101 | 150430 | 4.79% | 0.558% |
| 20 | 18.348 | 2854 | 2858 | 2868 | rVB | 556824 | 611304 | 19.47% | 2.267% |
| 21 | 19.065 | 2977 | 2980 | 2986 | rBV3 | 25095 | 40872 | 1.30% | 0.152% |
| 22 | 19.789 | 3096 | 3103 | 3110 | rBV2 | 43219 | 93320 | 2.97% | 0.346% |
| 23 | 20.012 | 3135 | 3141 | 3149 | rBV | 456759 | 596503 | 18.99% | 2.212% |
| 24 | 20.289 | 3185 | 3188 | 3194 | rBV8 | 19650 | 39350 | 1.25% | 0.146% |
| 25 | 20.641 | 3245 | 3248 | 3252 | rBV | 27158 | 34125 | 1.09% | 0.127% |
| 26 | 21.053 | 3313 | 3318 | 3324 | rBV8 | 20332 | 45030 | 1.43% | 0.167% |
| 27 | 21.594 | 3404 | 3410 | 3417 | rBV8 | 64659 | 165612 | 5.27% | 0.614% |
| 28 | 21.677 | 3420 | 3424 | 3428 | rBV7 | 17064 | 31852 | 1.01% | 0.118% |
| 29 | 21.794 | 3440 | 3444 | 3452 | rVB7 | 27745 | 62239 | 1.98% | 0.231% |
| 30 | 21.883 | 3456 | 3459 | 3465 | rVB7 | 21694 | 37000 | 1.18% | 0.137% |
| 31 | 22.330 | 3531 | 3535 | 3544 | rVB8 | 39327 | 76725 | 2.44% | 0.285% |
| 32 | 22.918 | 3628 | 3635 | 3647 | rVB7 | 79685 | 219543 | 6.99% | 0.814% |
| 33 | 23.053 | 3650 | 3658 | 3668 | rVB6 | 135743 | 361902 | 11.52% | 1.342% |

LSC Area Percent Report

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

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-BF060517.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

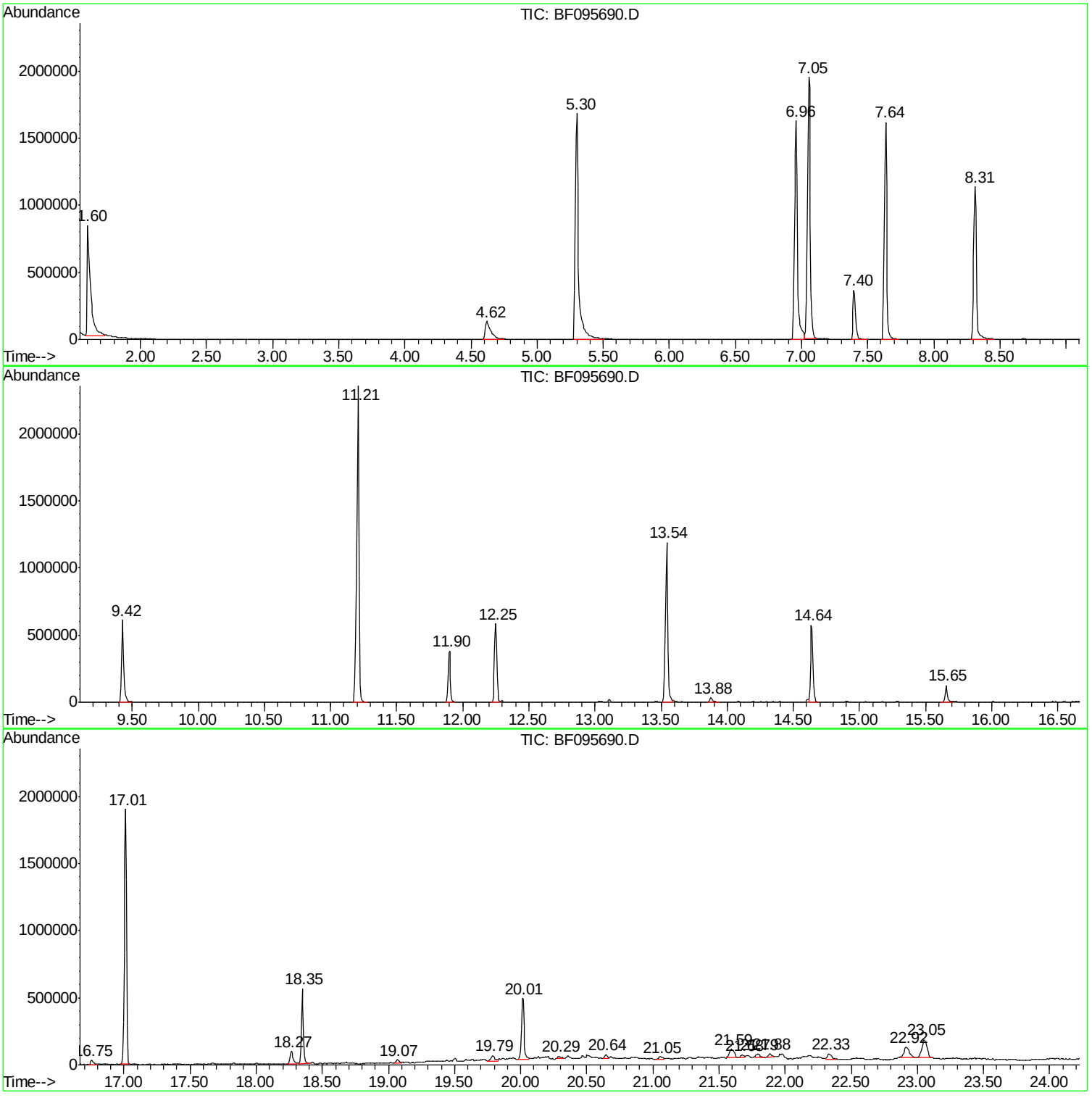
Sum of corrected areas: 26961934

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :**
BNA_F
**ClientSampleId :**
FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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\BF060517\
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Operator : SJ/MA
Sample : I3462-01
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ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

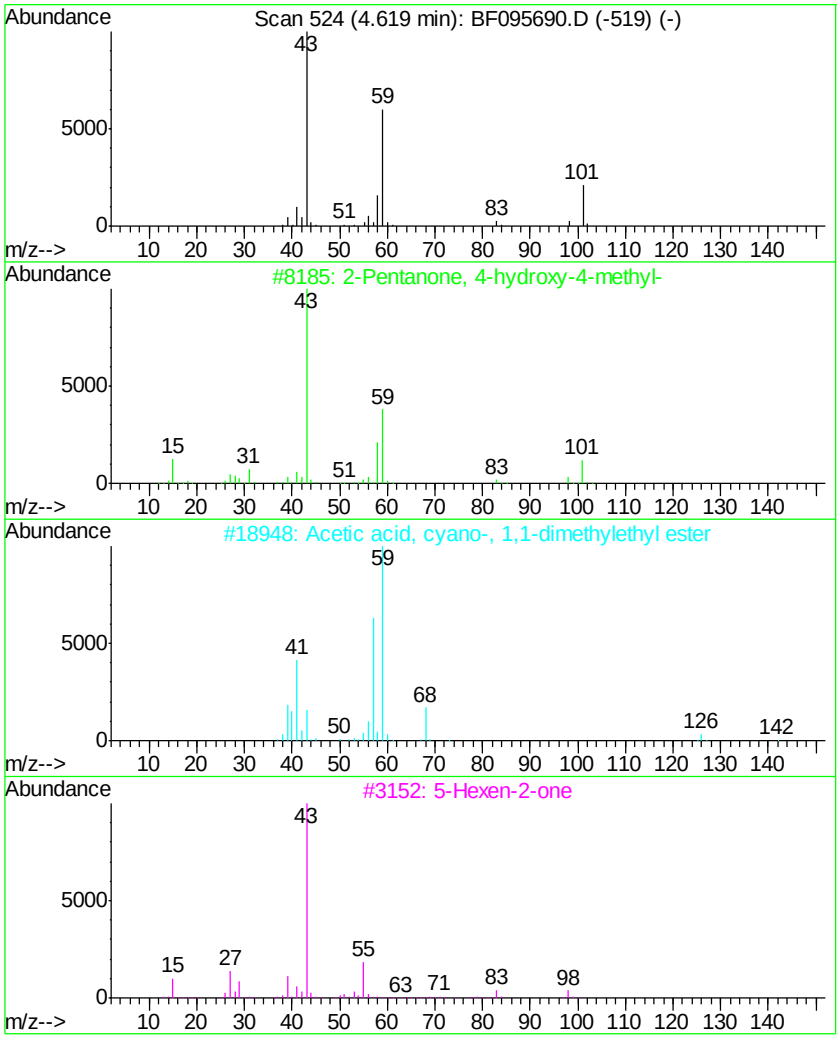
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

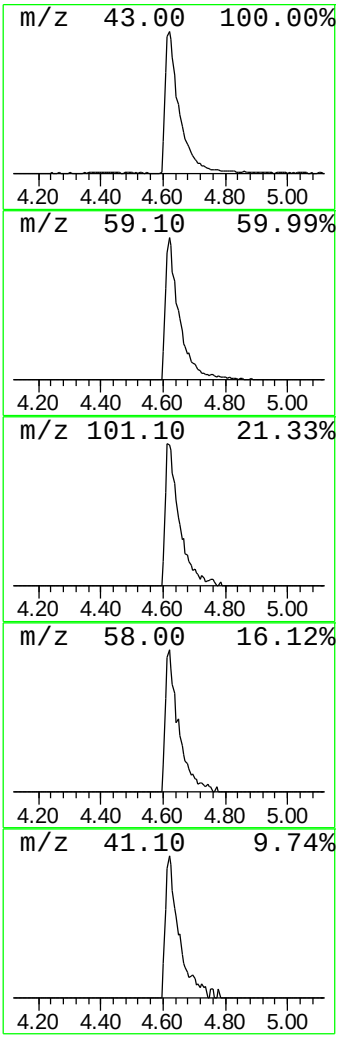
**********

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

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 4.62 | 16.89 ng | 413355 | 1,4-Dichlorobenzene-d4 | 7.40 |

| 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 | 25 |
| 3 | 5-Hexen-2-one | 98 | C6H10O | 000109-49-9 | 9 |
| 4 | Morpholine, 4-methyl- | 101 | C5H11NO | 000109-02-4 | 9 |
| 5 | 1,2-Butanediol | 90 | C4H10O2 | 000584-03-2 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

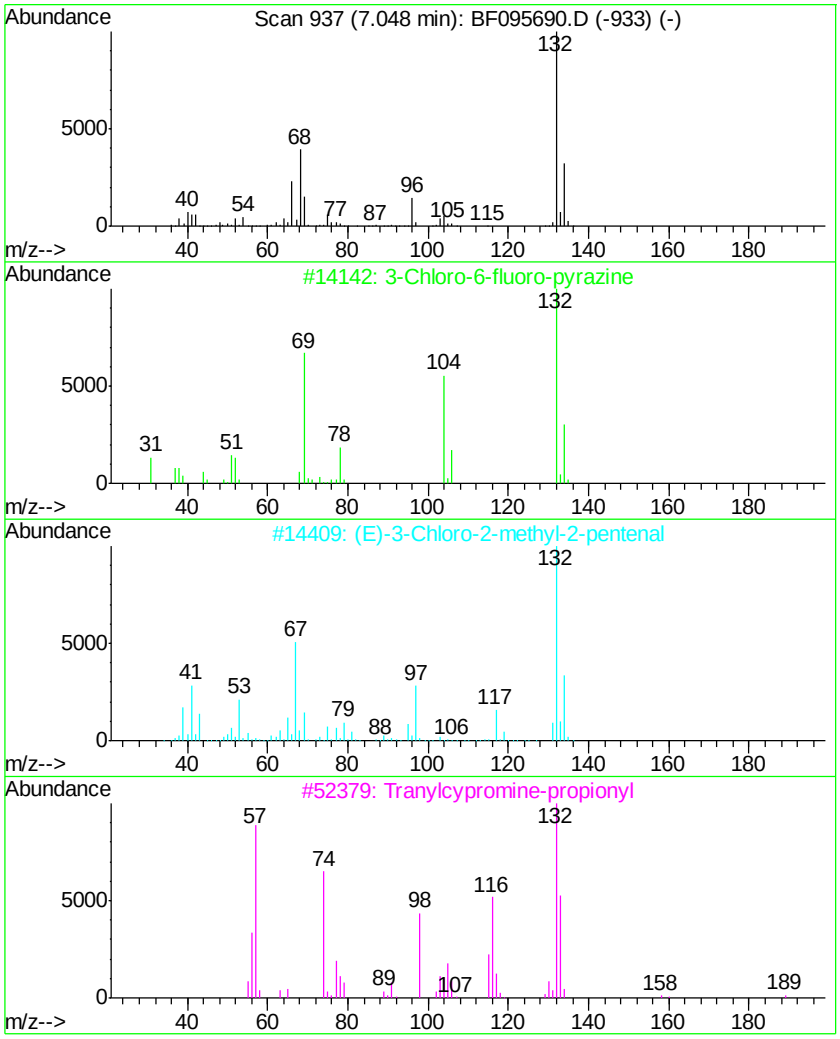
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

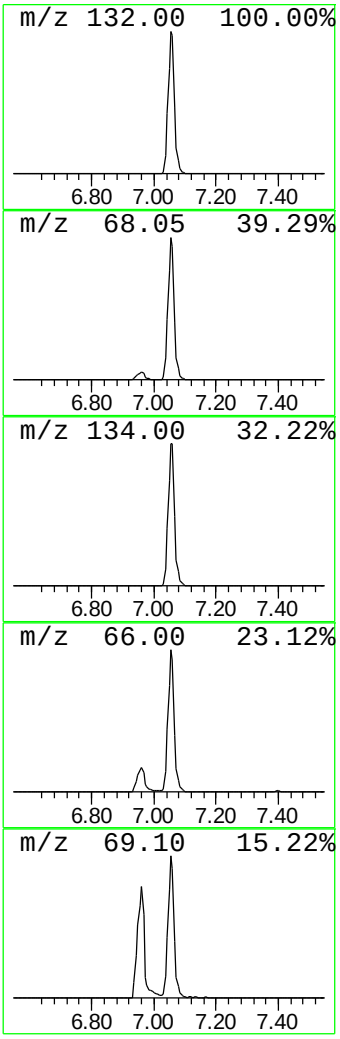
**********

Peak Number 3 unknown7.05 Concentration Rank 1

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 7.05 | 114.70 ng | 2807030 | 1,4-Dichlorobenzene-d4 | 7.40 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-Chloro-6-fluoro-pyrazine | 132 | C4H2ClFN2 | 1000146-10-7 | 27 |
| 2 | (E)-3-Chloro-2-methyl-2-pentenal | 132 | C6H9ClO | 031357-76-3 | 27 |
| 3 | Tranylcypromine-propionyl | 189 | C12H15NO | 1000123-86-3 | 10 |
| 4 | 5-Fluoro-2-chloropyrimidine | 132 | C4H2ClFN2 | 062802-42-0 | 9 |
| 5 | 1-Methylpyrrolo[1,2-a]pyrazine | 132 | C8H8N2 | 064608-59-9 | 9 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

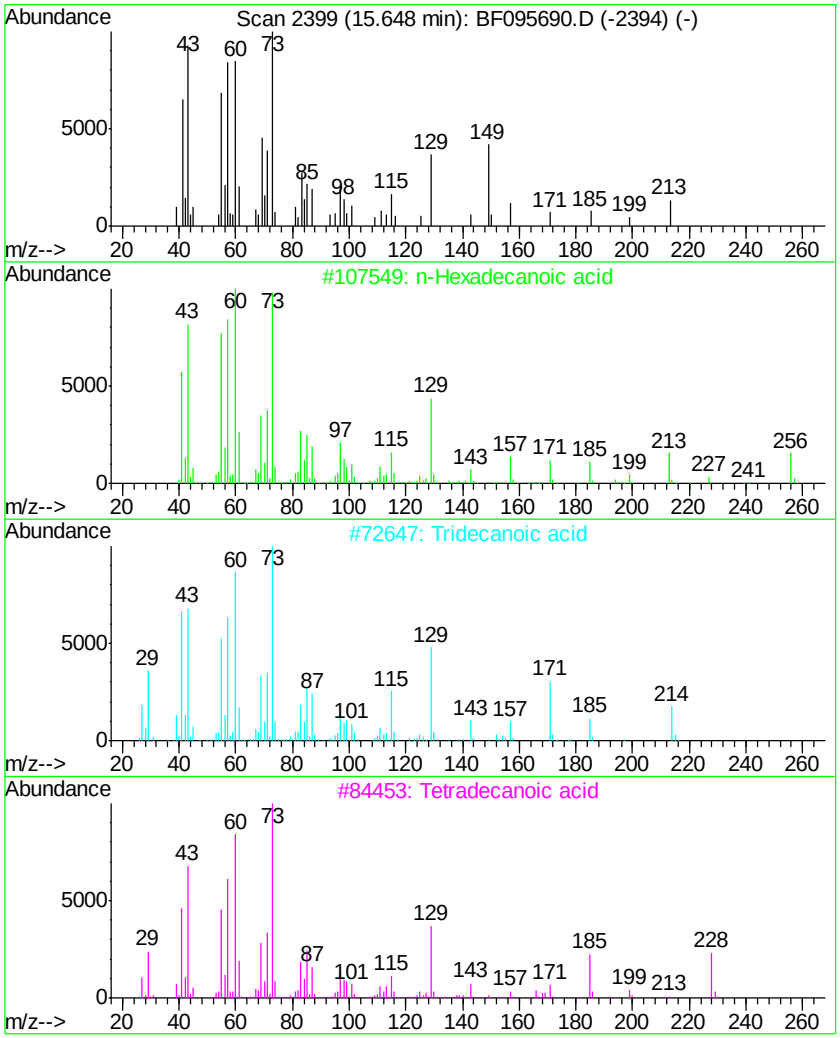
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

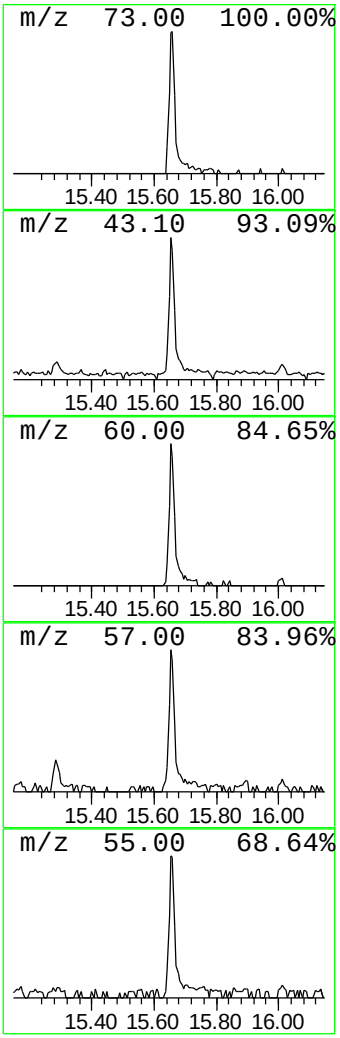
**********

Peak Number 5 n-Hexadecanoic acid Concentration Rank 9

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 15.65 | 4.52 ng | 165844 | Phenanthrene-d10 | 14.64 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | n-Hexadecanoic acid | 256 | C16H32O2 | 000057-10-3 | 97 |
| 2 | Tridecanoic acid | 214 | C13H26O2 | 000638-53-9 | 94 |
| 3 | Tetradecanoic acid | 228 | C14H28O2 | 000544-63-8 | 72 |
| 4 | Pentadecanoic acid | 242 | C15H30O2 | 001002-84-2 | 68 |
| 5 | Oxalic acid, isobutyl tetradecyl... | 342 | C20H38O4 | 1000309-37-9 | 18 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

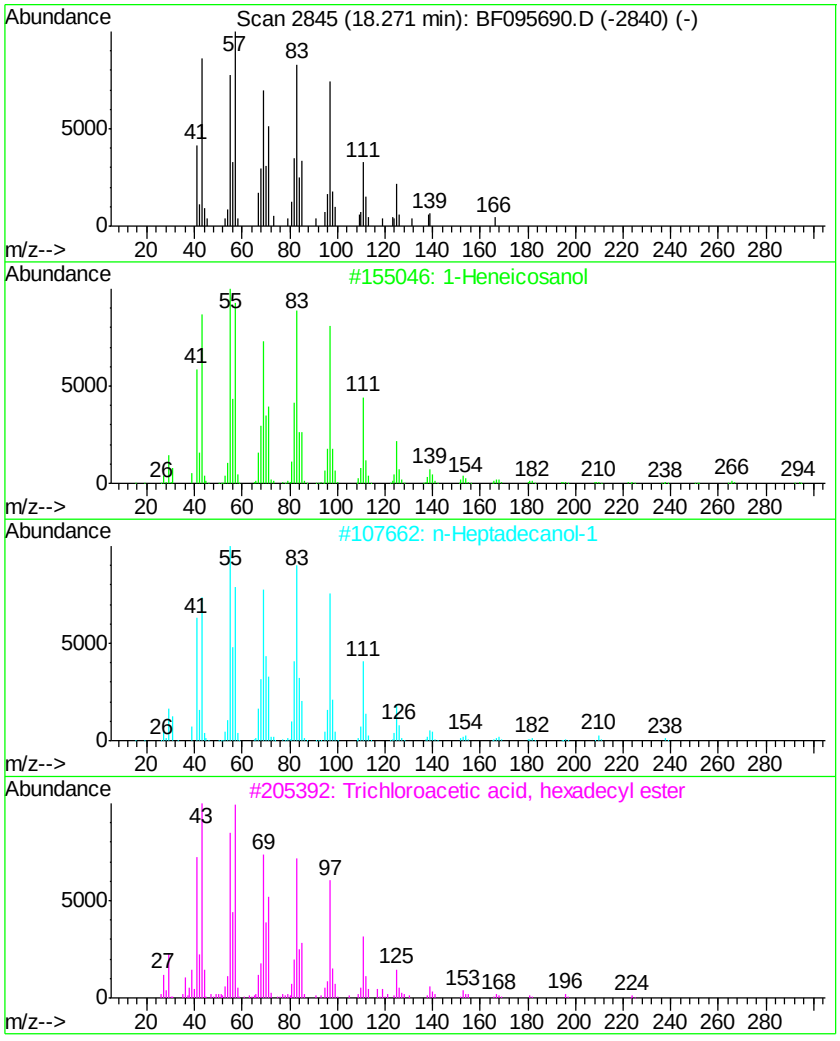
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

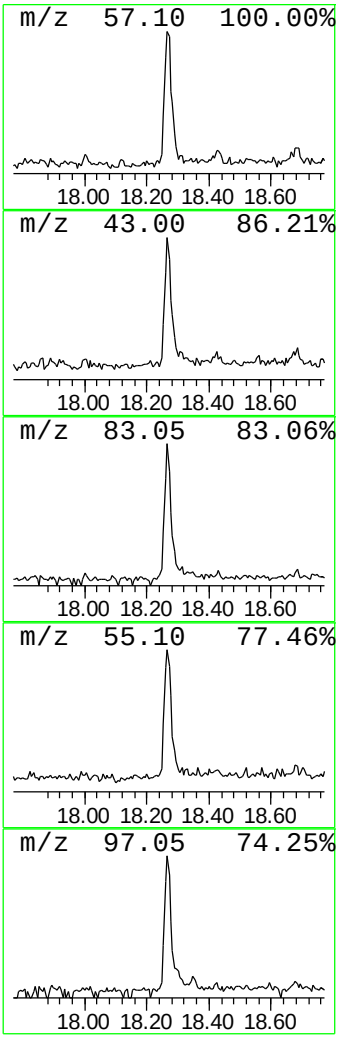
**********

Peak Number 6 1-Heneicosanol Concentration Rank 8

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 18.27 | 4.92 ng | 150430 | Chrysene-d12 | 18.35 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1-Heneicosanol | 312 | C21H44O | 015594-90-8 | 94 |
| 2 | n-Heptadecanol-1 | 256 | C17H36O | 001454-85-9 | 91 |
| 3 | Trichloroacetic acid, hexadecyl ... | 386 | C18H33Cl3O2 | 074339-54-1 | 90 |
| 4 | 3-Chloropropionic acid, heptadec... | 346 | C20H39ClO2 | 1000283-05-1 | 90 |
| 5 | n-Tetracosanol-1 | 354 | C24H50O | 000506-51-4 | 87 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

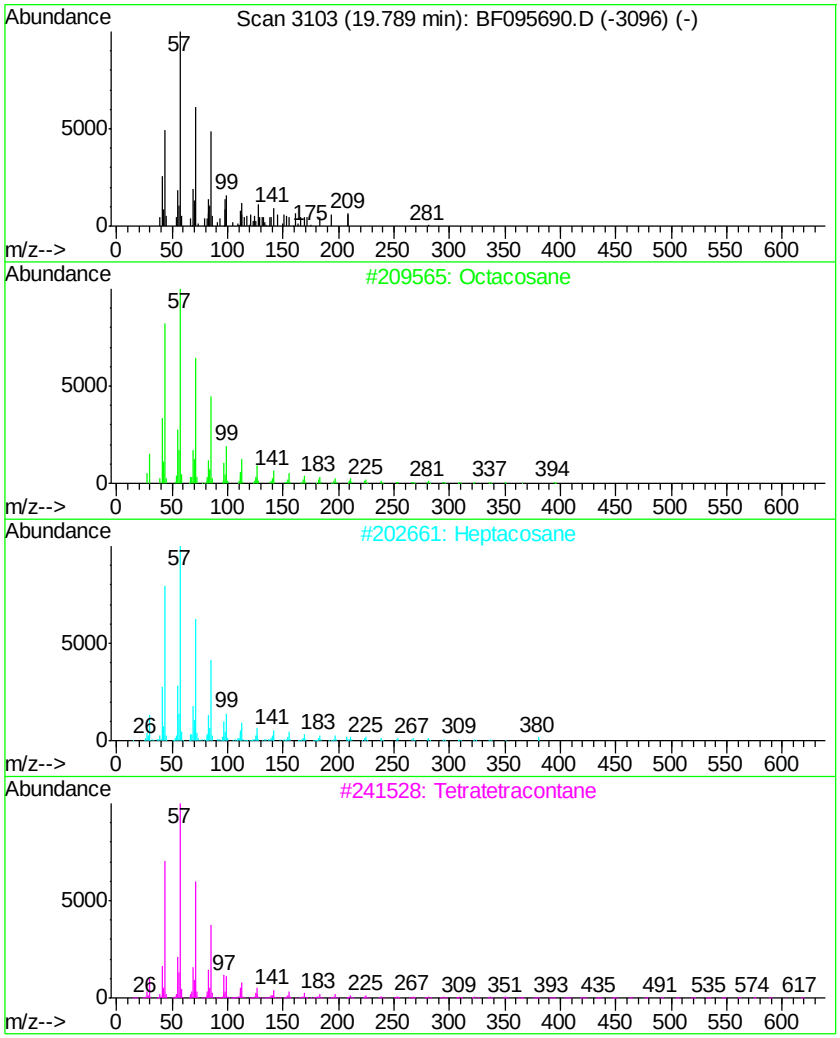
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

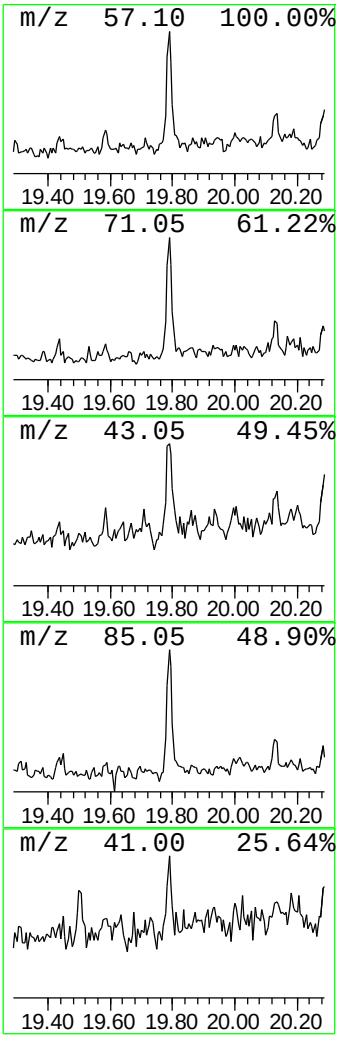
**********

Peak Number 7 Octacosane Concentration Rank 10

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 19.79 | 3.13 ng | 93320 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | Octacosane | 394 | C28H58 | 000630-02-4 | 91 |
| 2 | Heptacosane | 380 | C27H56 | 000593-49-7 | 91 |
| 3 | Tetratetracontane | 619 | C44H90 | 007098-22-8 | 90 |
| 4 | Hexatriacontane | 507 | C36H74 | 000630-06-8 | 90 |
| 5 | 2-methyltetracosane | 352 | C25H52 | 1000376-72-6 | 90 |



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Data File : BF095690.D
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Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

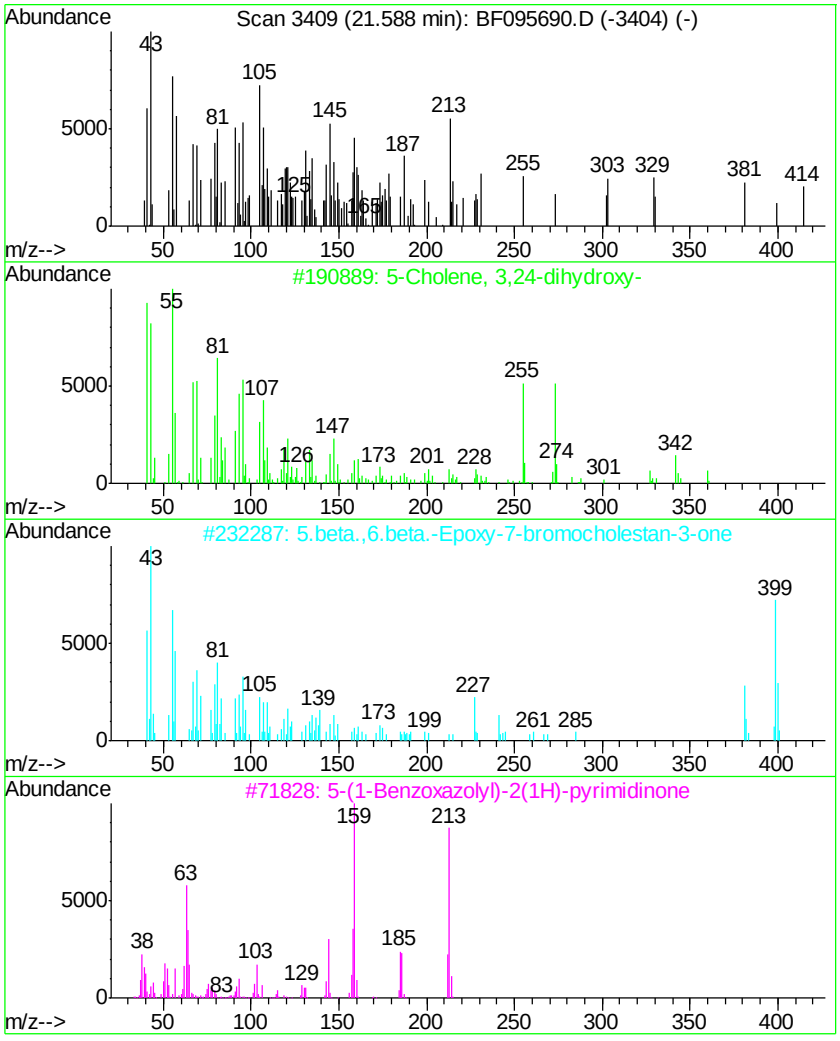
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

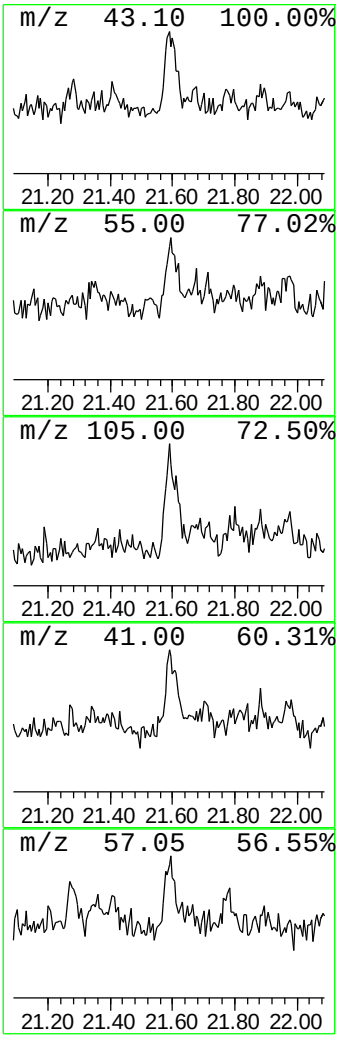
**********

Peak Number 8 unknown21.59 Concentration Rank 7

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.59 | 5.55 ng | 165612 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Cholene, 3,24-dihydroxy- | 360 | C24H40O2 | 1000251-69-2 | 22 |
| 2 | 5.beta.,6.beta.-Epoxy-7-bromocho... | 478 | C27H43BrO2 | 104825-82-3 | 14 |
| 3 | 5-(1-Benzoxazolyl)-2(1H)-pyrimid... | 213 | C11H7N3O2 | 349488-95-5 | 10 |
| 4 | Butanoic acid, carbonitrile, 2-(... | 205 | C10H8FN3O | 1000264-41-0 | 10 |
| 5 | .beta.-Sitosterol acetate | 456 | C31H52O2 | 000915-05-9 | 10 |



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**Instrument :** BNA_F
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

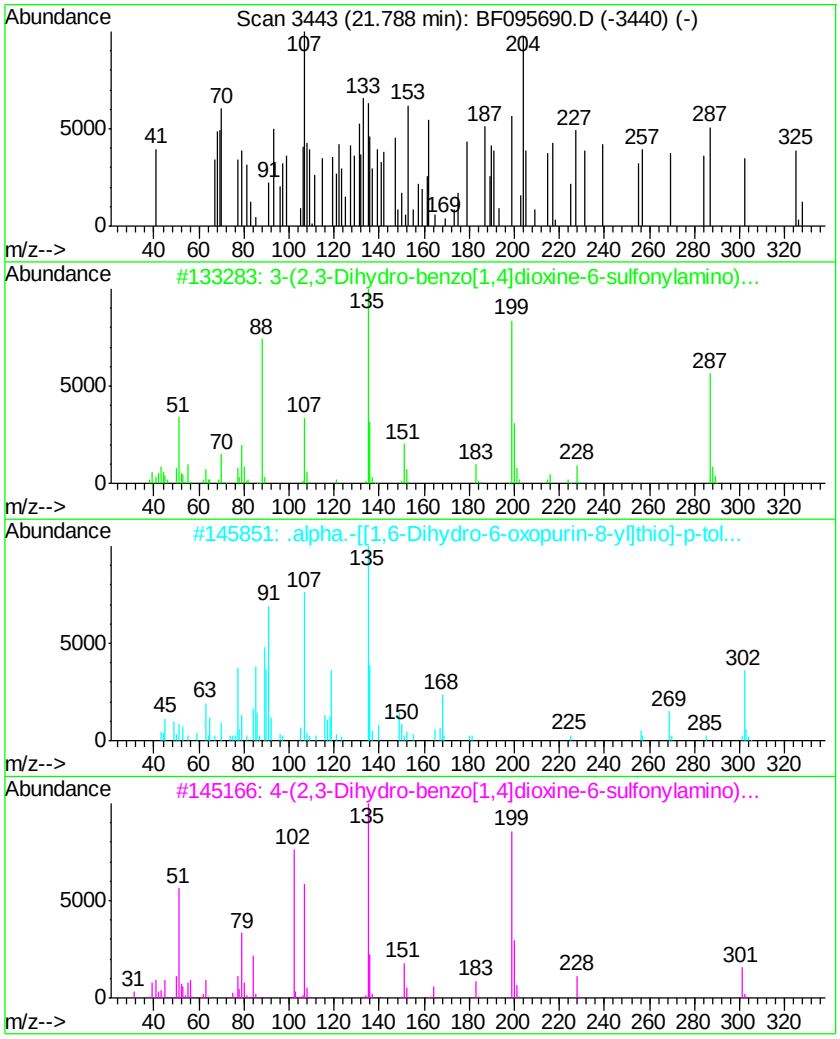
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

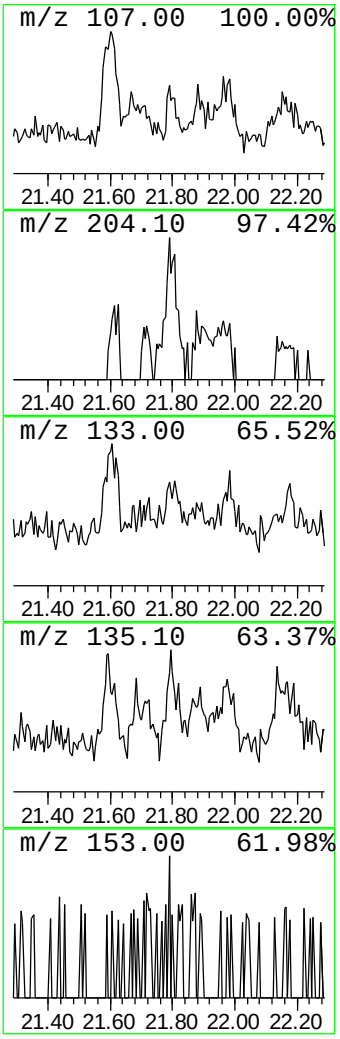
**********

Peak Number 9 unknown21.79 Concentration Rank 12

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 21.79 | 2.09 ng | 62239 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 3-(2,3-Dihydro-benzo[1,4]dioxine... | 287 | C11H13NO6S | 1000318-14-7 | 30 |
| 2 | .alpha.-[[1,6-Dihydro-6-oxopurin... | 302 | C13H10N4O3S | 1000213-14-9 | 30 |
| 3 | 4-(2,3-Dihydro-benzo[1,4]dioxine... | 301 | C12H15NO6S | 1000317-98-5 | 25 |
| 4 | Phosphonic acid, [1-methyl-1-[[[... | 328 | C15H25N2O4P | 1000350-82-9 | 22 |
| 5 | 1H-3a,7-Methanoazulene, 2,3,6,7,... | 204 | C15H24 | 000560-32-7 | 15 |



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ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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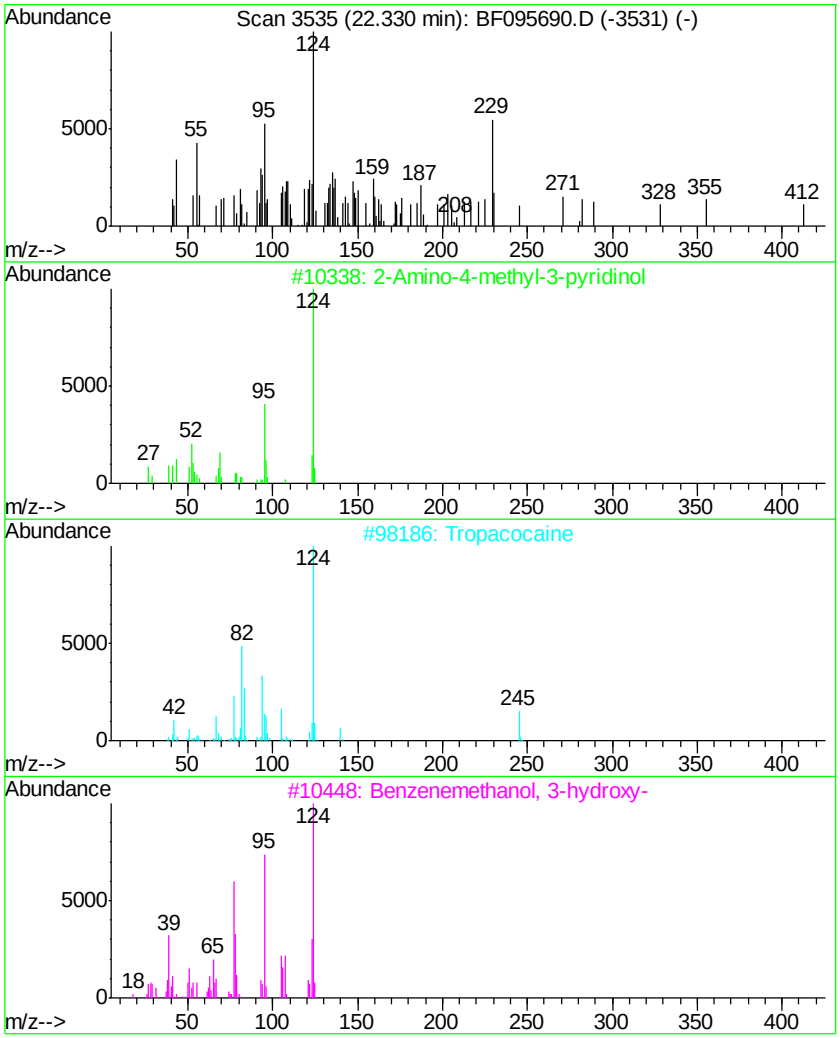
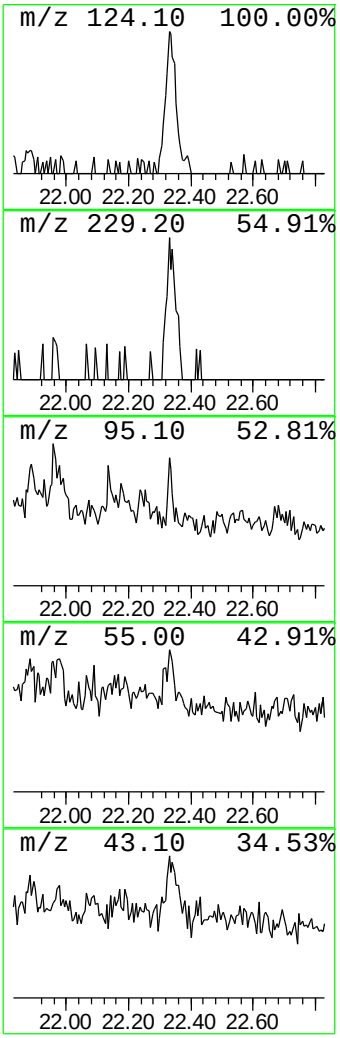
Peak Number 10 unknown22.33 Concentration Rank 11

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.33 | 2.57 ng | 76725 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 2-Amino-4-methyl-3-pyridinol | 124 | C6H8N2O | 020348-18-9 | 43 |
| 2 | Tropacocaine | 245 | C15H19NO2 | 000537-26-8 | 38 |
| 3 | Benzenemethanol, 3-hydroxy- | 124 | C7H8O2 | 000620-24-6 | 38 |
| 4 | Acetamide, 2-[2-(5-methylfuran-2... | 289 | C15H15NO3S | 1000259-79-3 | 38 |
| 5 | Pyrazine, 2-methoxy-5-(2-methylp... | 166 | C9H14N2O | 036330-05-9 | 27 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
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Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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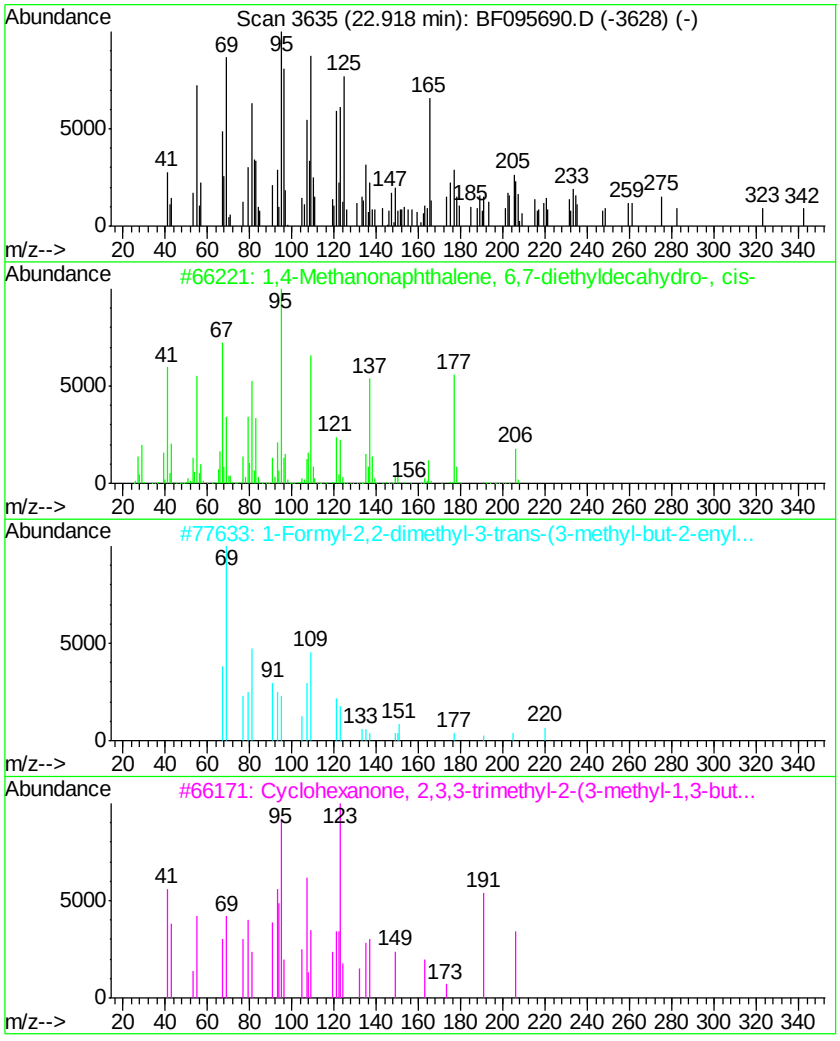
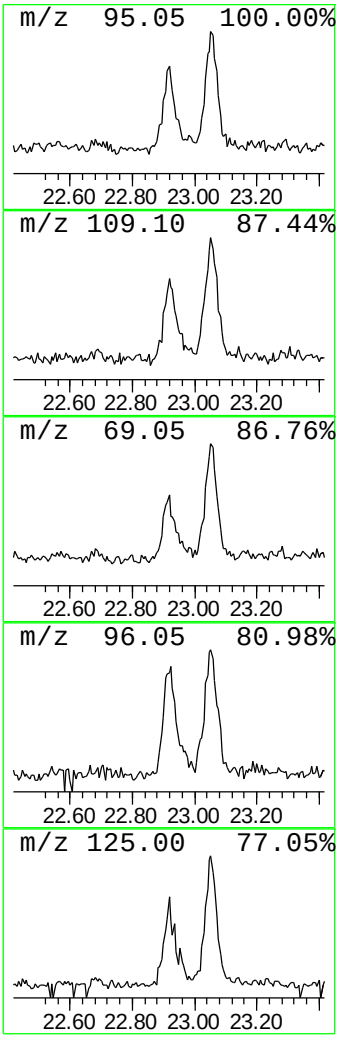
Peak Number 11 unknown22.92 Concentration Rank 6

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 22.92 | 7.36 ng | 219543 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 1,4-Methanonaphthalene, 6,7-diet... | 206 | C15H26 | 016539-02-9 | 27 |
| 2 | 1-Formyl-2,2-dimethyl-3-trans-(3... | 220 | C15H24O | 1000144-09-7 | 27 |
| 3 | Cyclohexanone, 2,3,3-trimethyl-2... | 206 | C14H22O | 069296-90-8 | 25 |
| 4 | 2-Hydroxy-6-methyl-6,7-dihydro-9... | 193 | C10H11NO3 | 1000210-15-9 | 22 |
| 5 | Pyrimidine, 4-amino-2-methoxy- | 125 | C5H7N3O | 003289-47-2 | 14 |



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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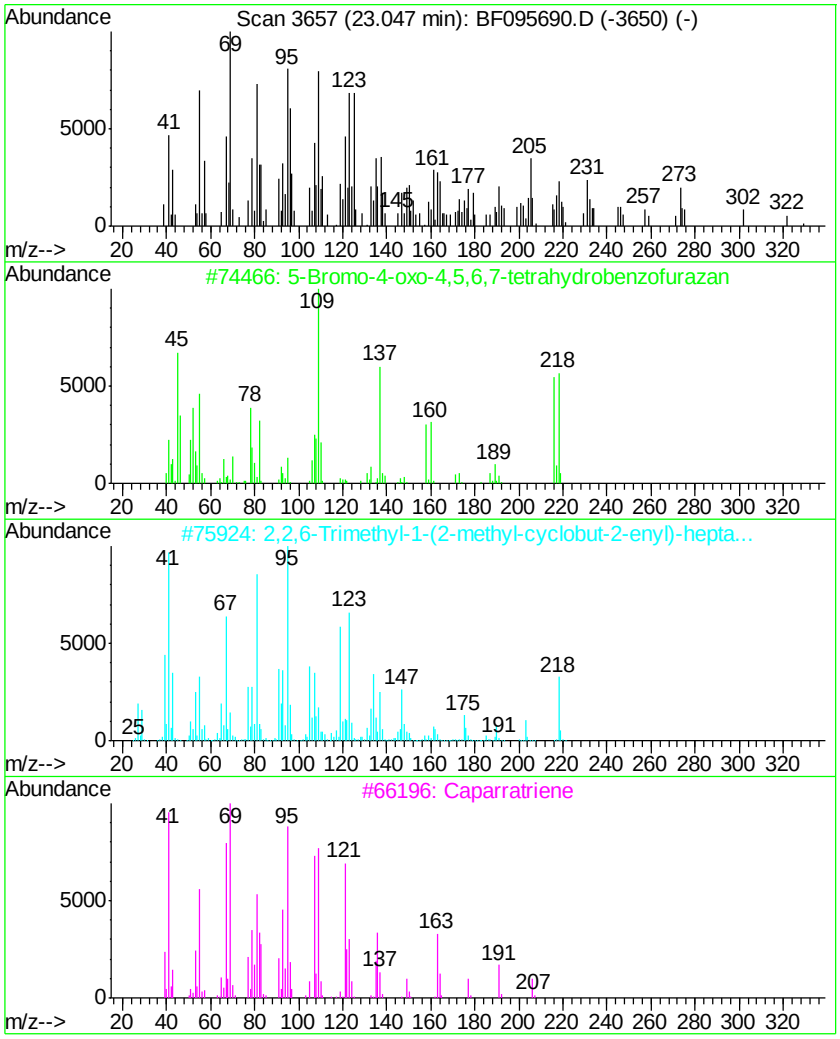
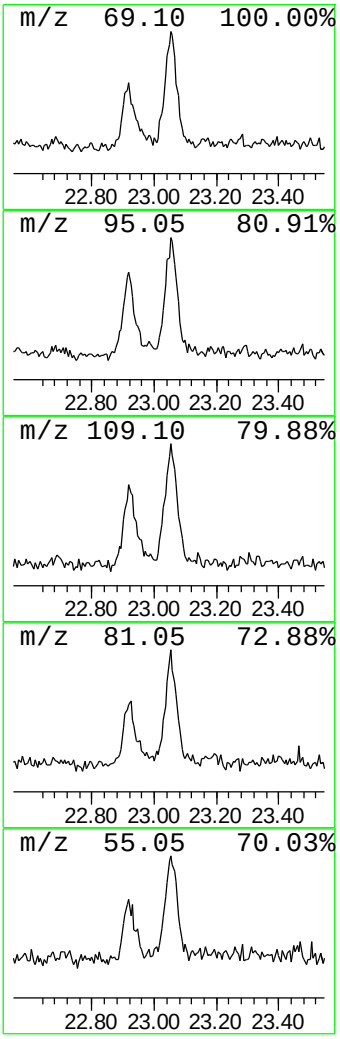
Peak Number 12 5-Bromo-4-oxo-4,5,6,7-tetra... Concentration Rank 5

| R.T. | EstConc | Area | Relative to ISTD | R.T. |
|---|---|---|---|---|
| 23.05 | 12.13 ng | 361902 | Perylene-d12 | 20.02 |

| Hit# of 5 | Tentative ID | MW | MolForm | CAS# | Qual |
|---|---|---|---|---|---|
| 1 | 5-Bromo-4-oxo-4,5,6,7-tetrahydro... | 216 | C6H5BrN2O2 | 300574-36-1 | 91 |
| 2 | 2,2,6-Trimethyl-1-(2-methyl-cycl... | 218 | C15H22O | 1000188-72-8 | 55 |
| 3 | Caparratriene | 206 | C15H26 | 1000374-08-7 | 49 |
| 4 | Bicyclo[2.2.1]heptane, 2,2,3-tri... | 138 | C10H18 | 020536-40-7 | 42 |
| 5 | Neopentylidenecyclohexane | 152 | C11H20 | 039546-80-0 | 42 |



Tentatively Identified Compound (LSC) summary

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF060517\
Data File : BF095690.D
Acq On : 6 Jun 2017 00:17
Operator : SJ/MA
Sample : I3462-01
Misc :
ALS Vial : 15 Sample Multiplier: 1

**Instrument :** BNA_F
**ClientSampleId :** FK-PS-01-005

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF060517.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... | 4.62 | 16.9 | ng | 413355 | 1 | 7.40 | 489456 | 20.0 |
| unknown7.05 | 7.05 | 114.7 | ng | 2807030 | 1 | 7.40 | 489456 | 20.0 |
| n-Hexadecanoic acid | 15.65 | 4.5 | ng | 165844 | 4 | 14.64 | 733597 | 20.0 |
| 1-Heneicosanol | 18.27 | 4.9 | ng | 150430 | 5 | 18.35 | 611304 | 20.0 |
| Octacosane | 19.79 | 3.1 | ng | 93320 | 6 | 20.02 | 596503 | 20.0 |
| unknown21.59 | 21.59 | 5.5 | ng | 165612 | 6 | 20.02 | 596503 | 20.0 |
| unknown21.79 | 21.79 | 2.1 | ng | 62239 | 6 | 20.02 | 596503 | 20.0 |
| unknown22.33 | 22.33 | 2.6 | ng | 76725 | 6 | 20.02 | 596503 | 20.0 |
| unknown22.92 | 22.92 | 7.4 | ng | 219543 | 6 | 20.02 | 596503 | 20.0 |
| 5-Bromo-4-oxo-4,5... | 23.05 | 12.1 | ng | 361902 | 6 | 20.02 | 596503 | 20.0 |